Supplementary Information (SI)

Extreme Multi-Point van der Waals Interaction: Isolable Dimers of Phthalocyanines Substituted with Pillar-like Azaacenes

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Contents:

General Information

All the purchased reagents were of standard quality, and used without further purification. ^{1}H NMR, ^{13}C NMR, ^{1}H/^{13}C HMQC, ^{1}H/^{13}C HMBC, ^{1}H-^{1}H COSY, and ^{1}H DPFGSE-NOE spectra were recorded by a JEOL JNM-AL400 FT-NMR, a JNM-ECZ500R, or a JNM-ECA600P instrument. Chemical shifts of NMR spectra are determined relative to corresponding solvent signal, and are given in parts per million (ppm). The asterisk marks in the NMR spectra represent the solvent residual peaks. Low and high resolution matrix-assisted-laser-desorption/ionization (MALDI) mass spectra (MS) were obtained on a Bruker ultraflex mass spectrometer with dithranol as a matrix. The separation of the monomeric and dimeric Pcs was performed using a high-pressure liquid chromatography system (JAI LC-9210 NEXT) with a size exclusion column (JAI JAIGEL-2.5/3HH). UV-Vis-NIR absorption spectra were obtained with a JASCO V-570 spectrometer. Electron spin resonance (ESR) spectra were recorded on a JEOL JES-TE200 X-band ESR spectrometer, in which temperature was controlled by a JEOL ES-DVT3 variable-temperature unit. A Mn^{2+}/MnO solid solution was used a reference. The redox properties were evaluated by cyclic voltammetry (CV) and differential pulse voltammetry (DPV) in CH_2Cl_2 solution at 298 K with 0.1 M tetra-*n*-butylammonium tetrafluoroborate ($TBABF_4$) as supporting electrolyte (scan rate 100 mV s^{-1}) using an ALS/chi Electrochemical Analyzer model 612A. A three-electrode assembly was used, which was equipped with platinum disk (2 mm^2), a platinum wire, and Ag/0.01 M $AgNO_3$ (acetonitrile) as the working electrode, the counter electrode, and the reference electrode, respectively. The redox potential were referenced against a ferrocene/ferrocenium ($Fc^{0/+}$) redox potential measured in the same electrolytic solution.

The activation energies of the association and dissociation of **1Zn** and **1Zn2** were evaluated from the temporal changes of the concentrations of **1Zn** and **1Zn2**. The concentrations of **1Zn** and **1Zn2** were estimated from the electronic absorption spectra of the solutions of **1Zn** and **1Zn2** as follows. During the electronic absorption measurements, the following two equations are established:

$$A_{Q1Zn} = \varepsilon_{1Zn\_at\_Q1Zn}[1Zn]l + \varepsilon_{1Zn2\_at\_Q1Zn}[1Zn2]l \quad (1)$$

$$[1Zn] + 2[1Zn2] = [1Zn]_{total} \quad (2)$$

The parameters are defined as follows.

A_{Q1Zn}: absorbance at the peak top wavelength of the Q-band of **1Zn**

$\varepsilon_{1Zn\_at\_Q1Zn}$ and $\varepsilon_{1Zn2\_at\_Q1Zn}$: molar extinction coefficient of **1Zn** and **1Zn2** at the peak top wavelength of the Q-band of **1Zn**

[**1Zn**] and [**1Zn2**]: concentration of **1Zn** and **1Zn2**

$[\mathbf{1Zn}]_{\mathrm{total}}$: total concentration of **1Zn** if all **1Zn2** molecules exist as **1Zn** (in this work, $[\mathbf{1Zn}]_{\mathrm{total}} = 1 \times 10^{-5}$ M)

l: path length of the optical cell (in this work, $l = 1$ cm)

The concentrations of **1Zn** (or **1Zn2**) were calculated by combining eq. 1 and eq. 2. The dissociation and dimerization reactions are assumed to be the first- and second-order reaction, respectively. The reverse reactions (the dissociation of **1Zn2** in ethyl acetate and the dimerization of **1Zn** in *o*-dichlorobenzene) were assumed to be negligibly slow judging from the fact that the spectra of **1Zn2** in ethyl acetate and of **1Zn** in *o*-dichlorobenzene showed no temporal changes.

Synthetic Details

1Zn2, **1Zn**: A mixture of **2** (200 mg, 0.23 mmol), zinc acetate (11 mg, 0.059 mmol), DBU (4 drops), in 1-pentanol (50 ml) was refluxed under a nitrogen atmosphere for 24 h. The reaction mixture was cooled down to room temperature and precipitated by adding methanol. The crude solid was filtered and chromatographed on HPLC (chloroform as eluent). The obtained partially oxidized product was reduced by hydrazine and washed with water to afford **1Zn2** (47 mg, 23%) and **1Zn** (6 mg, 3%) as green solid. **1Zn**; ^{1}H NMR (400 MHz, tetrahydrofuran-d_8) δ = 1.00 (t, J = 6.34 Hz, 24H), 1.51 (m, 64H), 3.55 (m), 6.36 (s, 16H), 6.44 (t, J = 7.31 Hz, 16H), 6.58 (d, J = 7.80 Hz, 16H), 6.65 (s, 16H), 6.73 (t, J = 7.31 Hz, 16H), 7.03 (d, J = 7.80 Hz, 16H), 10.27 (s, 8H); ^{13}C NMR (100 MHz, tetrahydrofuran-d_8) δ = 14.41, 23.66, 25.13, 27.46, 32.61, 46.74, 106.60, 111.15, 123.40, 124.01, 125.93, 126.24, 130.24, 131.91, 131.97, 135.07, 135.19, 139.76, 141.56, 155.12; MALDI HRMS (dithranol): calculated monoisotopic mass for $C_{240}H_{208}N_{24}Zn$ 3489.630 $[M]^+$; found 3489.619; MALDI MS (dithranol): calculated molecular weight for $C_{240}H_{208}N_{24}Zn$ 3493.85; found 3493.1 $[M]^+$. **1Zn2**; ^{1}H NMR (400 MHz, tetrahydrofuran-d_8) δ = 0.96 (t, J = 6.83 Hz, 48H), 1.24 (br, 64H), 1.35 (br, 64H), 2.73 (brs, 16H), 2.90 (brs, 16H), 5.66 (s, 32H), 5.88 (s, 16H), 5.94 (t, J = 7.31 Hz, 16H), 6.16 (brs, 16H), 6.36 (t, J = 7.31 Hz, 32H), 6.57 (d, J = 7.80 Hz, 16H), 6.74 (t, J = 7.31 Hz, 16H), 7.01 (d, J = 7.80 Hz, 16H), 7.37 (brs, 16H), 7.67 (s, 16H), 10.27 (s, 16H); ^{13}C NMR (100 MHz, tetrahydrofuran-d_8) δ = 14.46, 23.65, 24.90, 27.34, 32.61, 46.15, 105.81, 105.93, 108.35, 112.32, 122.67, 122.89, 123.08, 123.46, 125.27, 125.61, 125.96, 126.63, 129.48, 130.05, 131.55, 131.67, 132.06, 133.48, 133.79, 134.44, 134.84, 139.42, 139.47, 155.60; MALDI MS (dithranol): calculated molecular weight for $C_{480}H_{416}N_{48}Zn_2$ 6987.704; found 6987.725 $[M]^+$ (Figure S3).

1Cu2, **1Cu** : A mixture of **2** (100 mg, 0.117 mmol), copper chloride (3.93 mg, 0.029 mmol), DBU (4 drops), in 1-pentanol (40 ml) was refluxed under a nitrogen atmosphere for 24 h. The reaction mixture was cooled down to room temperature and precipitated with methanol. The crude solid was filtered and chromatographed on HPLC (chloroform as eluent). The obtained partially oxidized product was reduced by hydrazine and washed with water to afford **1Cu2** (21 mg, 21%) and **1Cu** (2mg, 2%) as green solid. **1Cu**; MALDI HRMS (dithranol): m/z calcd monoisotopic mass for $C_{240}H_{208}N_{24}Cu$ 3488.630 $[M]^+$; found 3488.623; MALDI MS: calculated monoisotopic mass for $C_{240}H_{208}N_{24}Cu$ 3492.02 ; found 3491.64 $[M]^+$ (Figure S3). **1Cu2** MALDI MS (dithranol): calculated molecular weight for $C_{480}H_{416}N_{48}Cu_2$ 6984.04; found 6983.83 $[M]^+$.

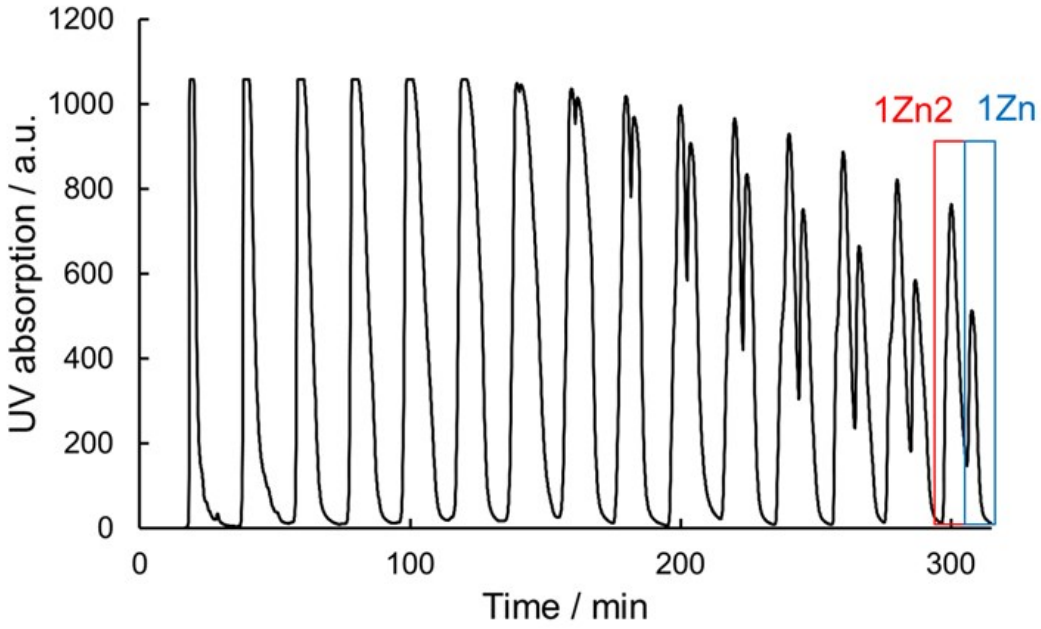

Figure S1. Recycling preparative gel permeation chromatogram of the reaction crude containing **1Zn** and **1Zn2** with chloroform as a mobile phase. Detection wavelength is 280 nm.

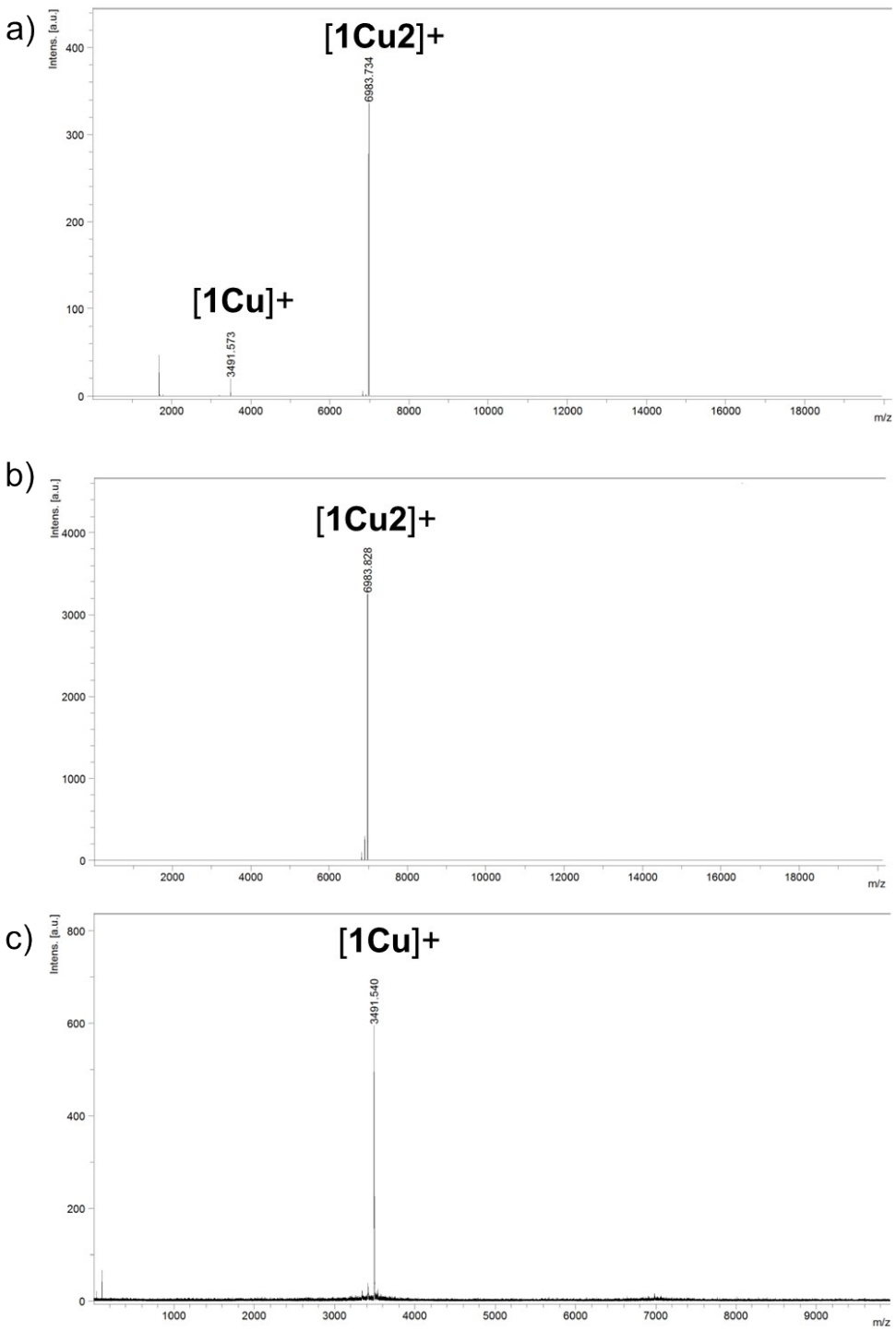

Figure S2. MALDI-TOF-MS spectra (positive) of **(**a) the reaction crude containing **1Cu** and **1Cu2** and of (b) **1Cu2** and (c) **1Cu** isolated by HPLC.

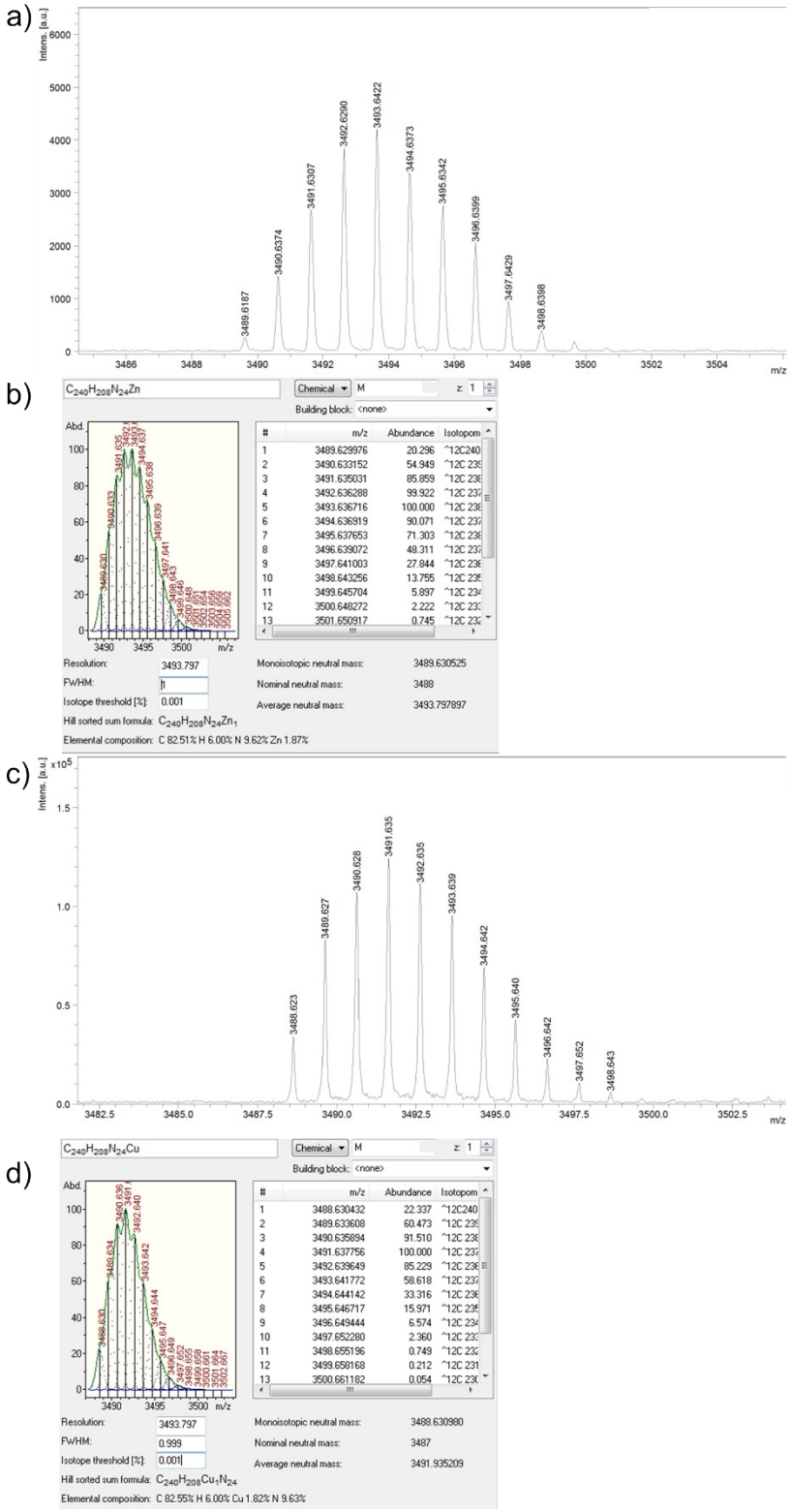

Figure S3. MALDI high-resolution mass spectra of **1Zn**: (a) experimental and (b) simulated (for $[M^+]$) and of **1Cu**: (c) experimental and (d) simulated (for $[M^+]$).

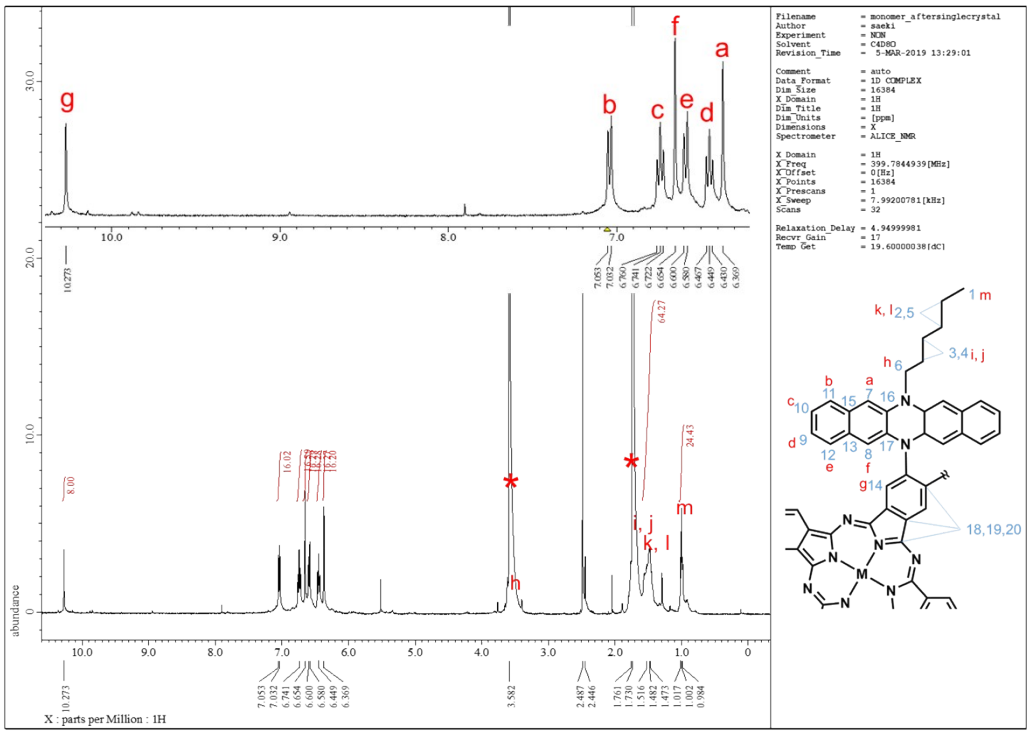

Figure S4. ^{1}H NMR spectra of **1Zn** at 298 K (tetrahydrofuran-d_8, 400 MHz).

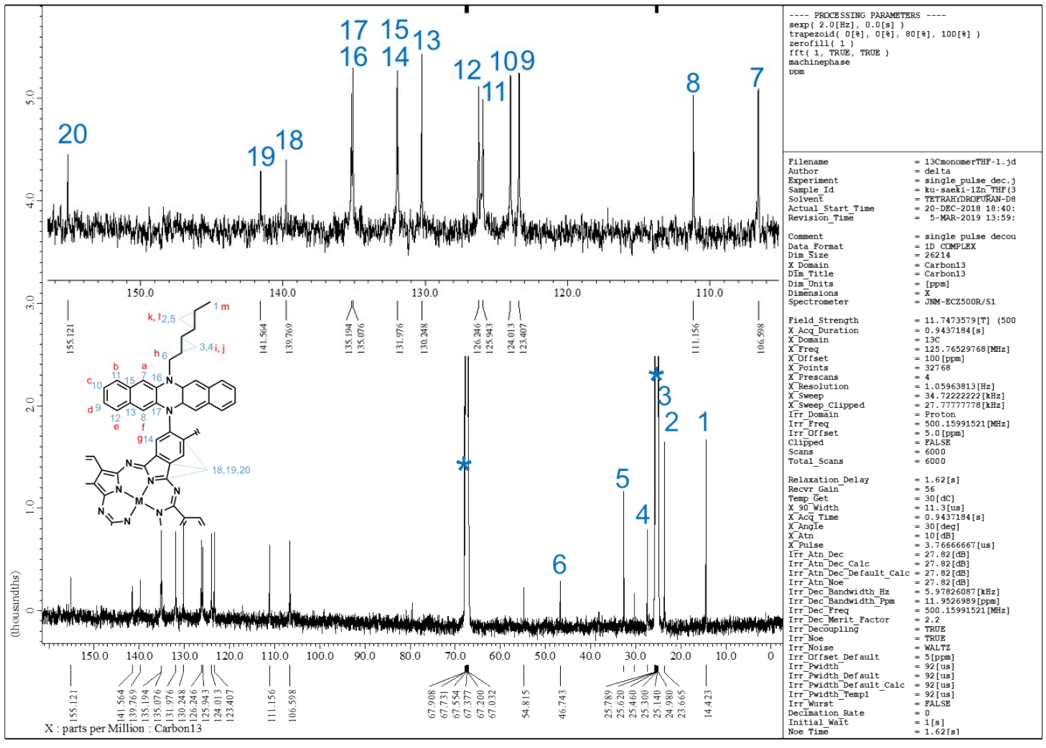

Figure S5. ^{13}C NMR spectra of **1Zn** at 303 K (tetrahydrofuran-d_8, 500 MHz).

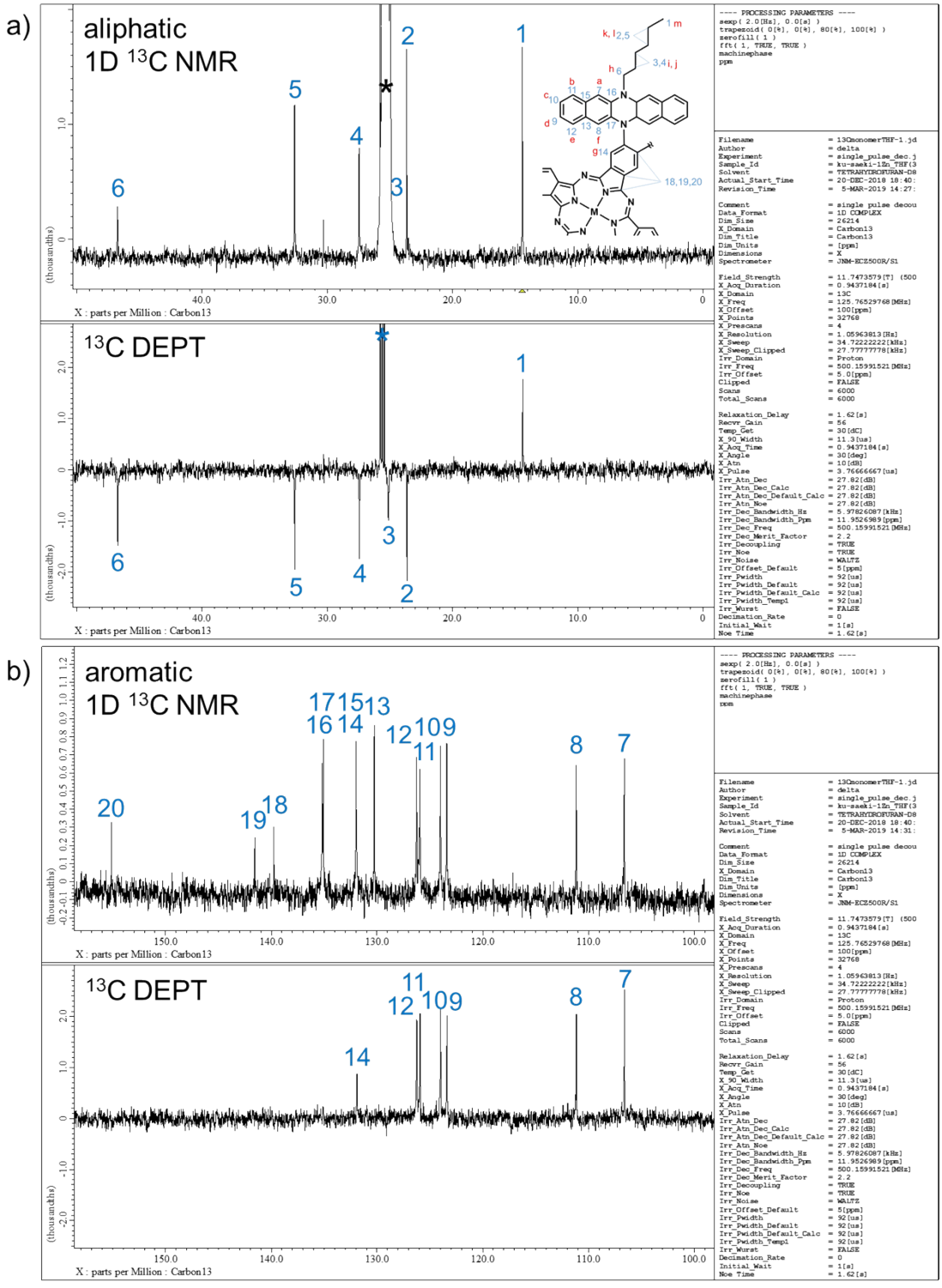

Figure S6. ^{13}C NMR and ^{13}C DEPT spectra of **1Zn** at 303 K. a) aliphatic region and b) aromatic region. (tetrahydrofuran-d_8, 500 MHz)

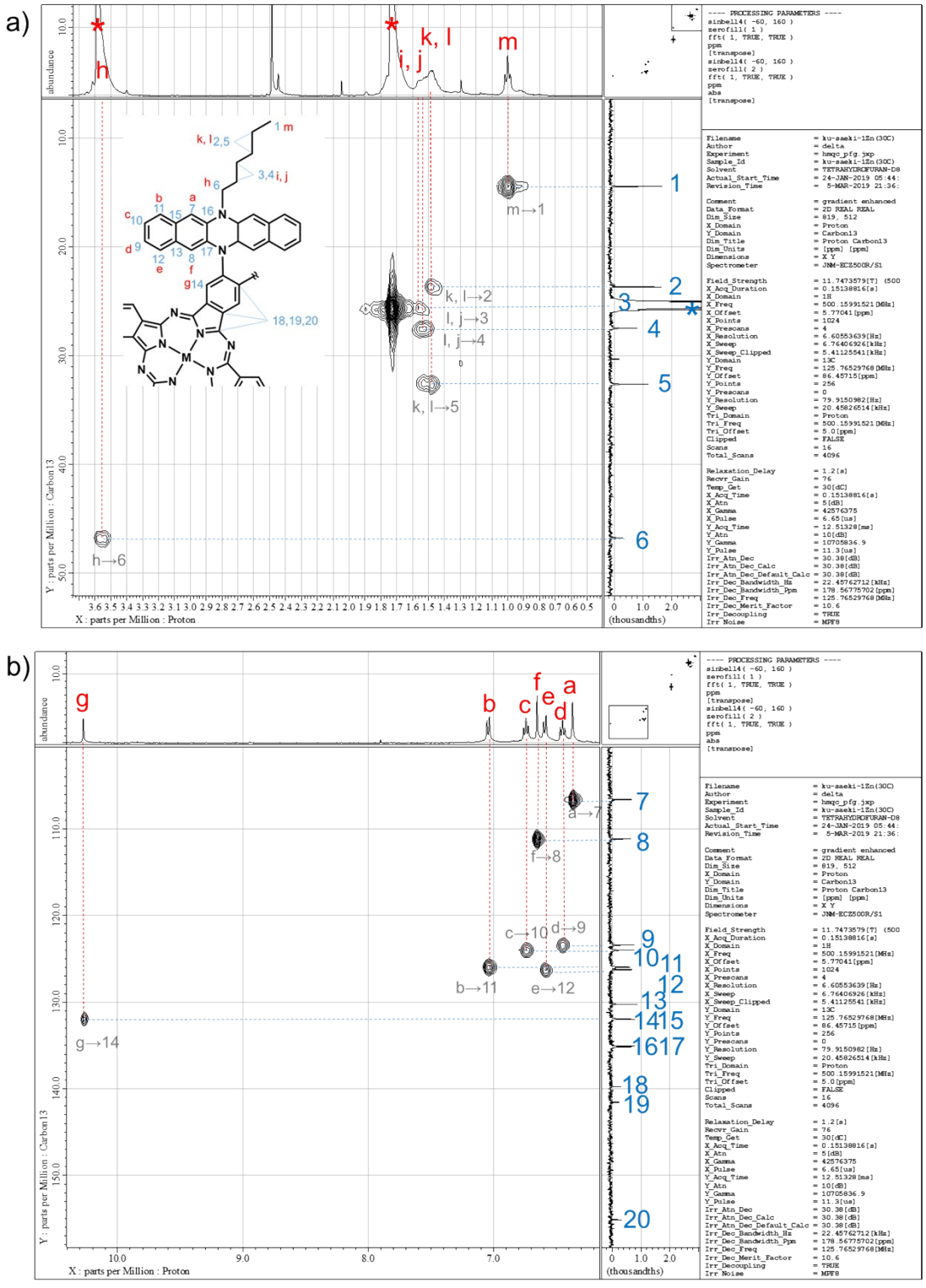

Figure S7. $^{13}C/^{1}H$ HMQC spectra of **1Zn** at 303 K. (a) aliphatic region and (b) aromatic region (tetrahydrofuran-d_8, 500 MHz).

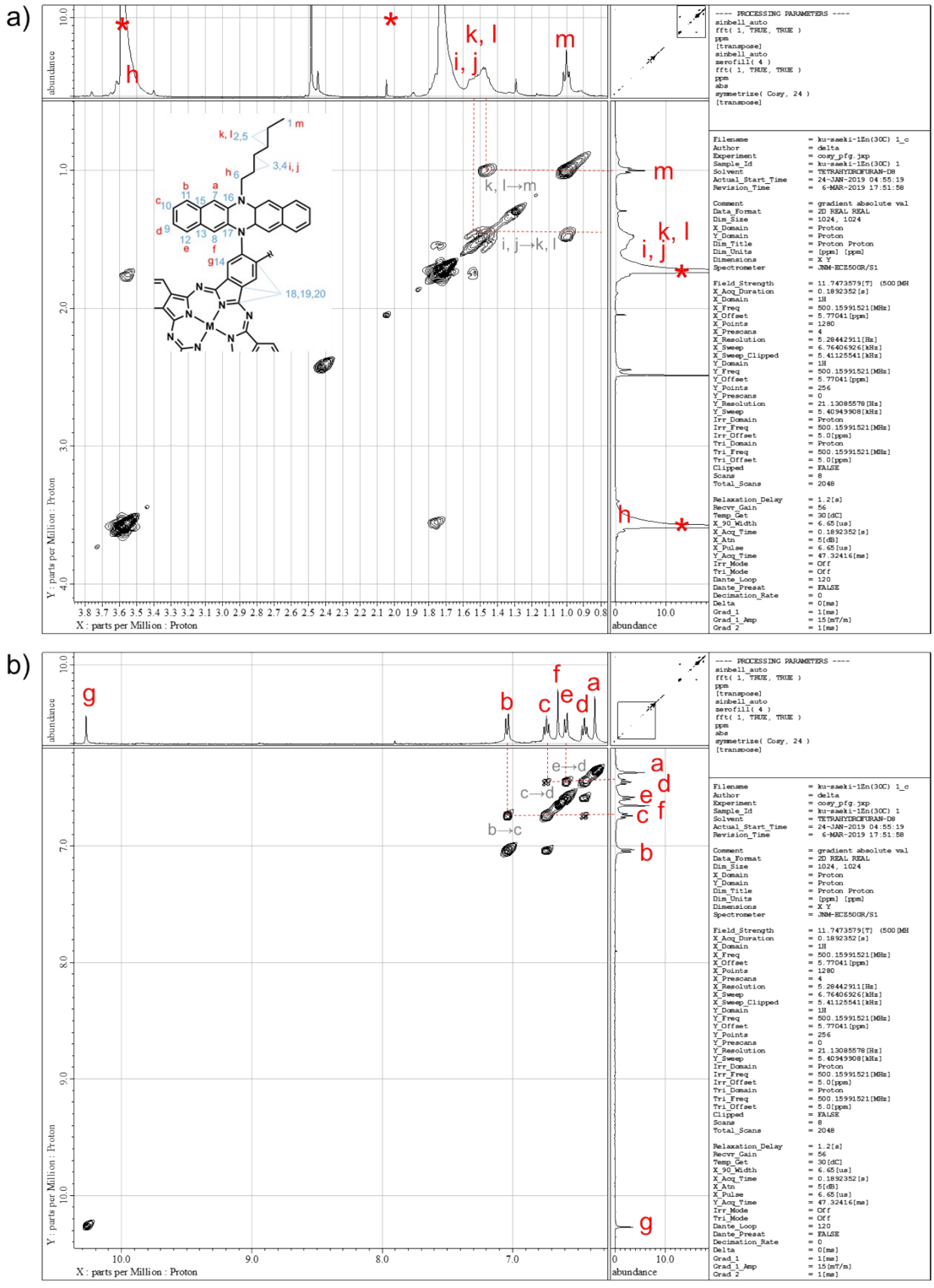

Figure S8. ^{1}H–^{1}H COSY spectra of **1Zn** at 303 K. (a) aliphatic region and (b) aromatic region (tetrahydrofuran-d_8, 500 MHz).

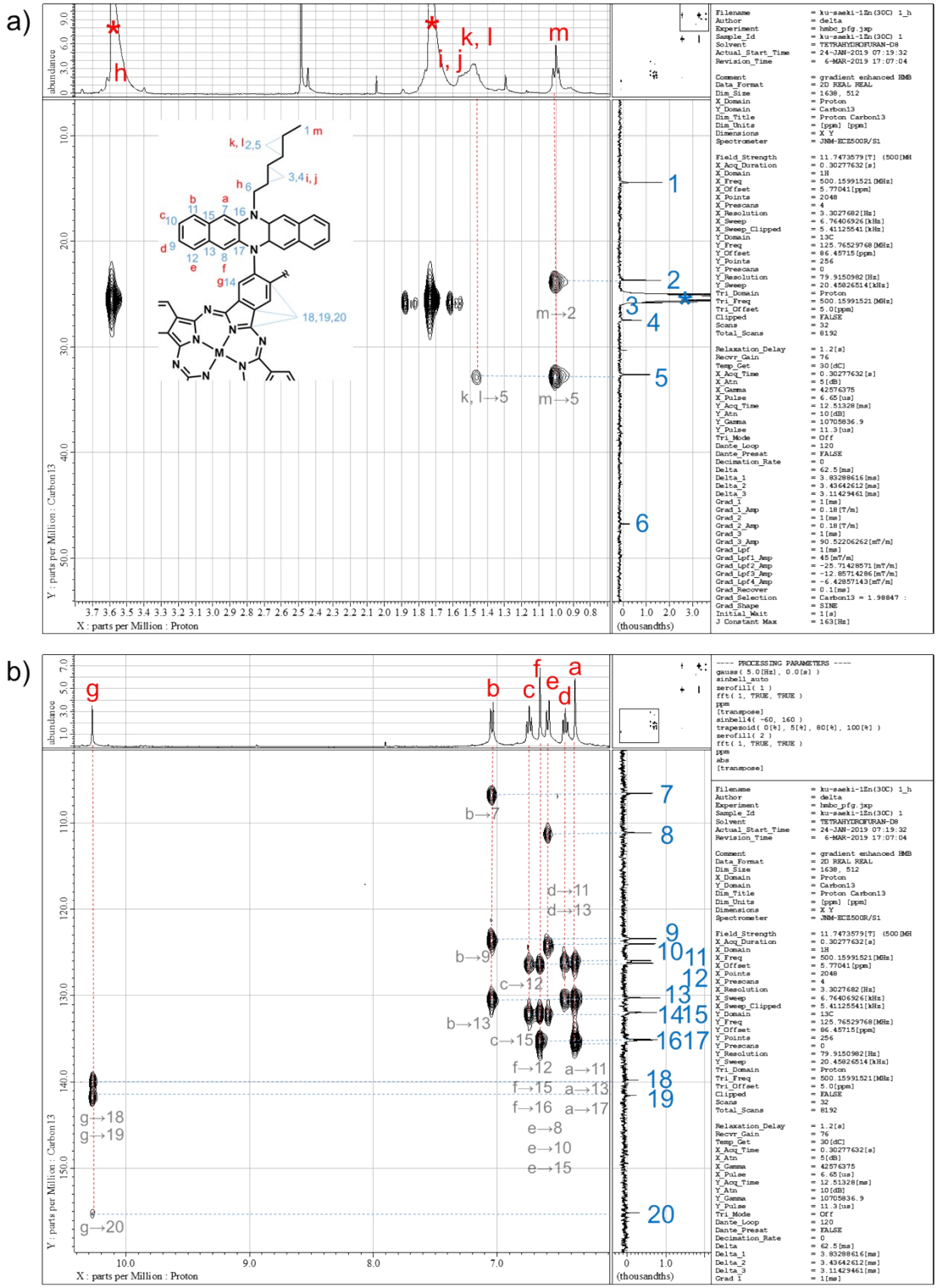

Figure S9. $^{13}C/^{1}H$ HMBC spectra of **1Zn** in tetrahydrofuran-d_8 at 303 K. (a) aliphatic region and (b) aromatic region.

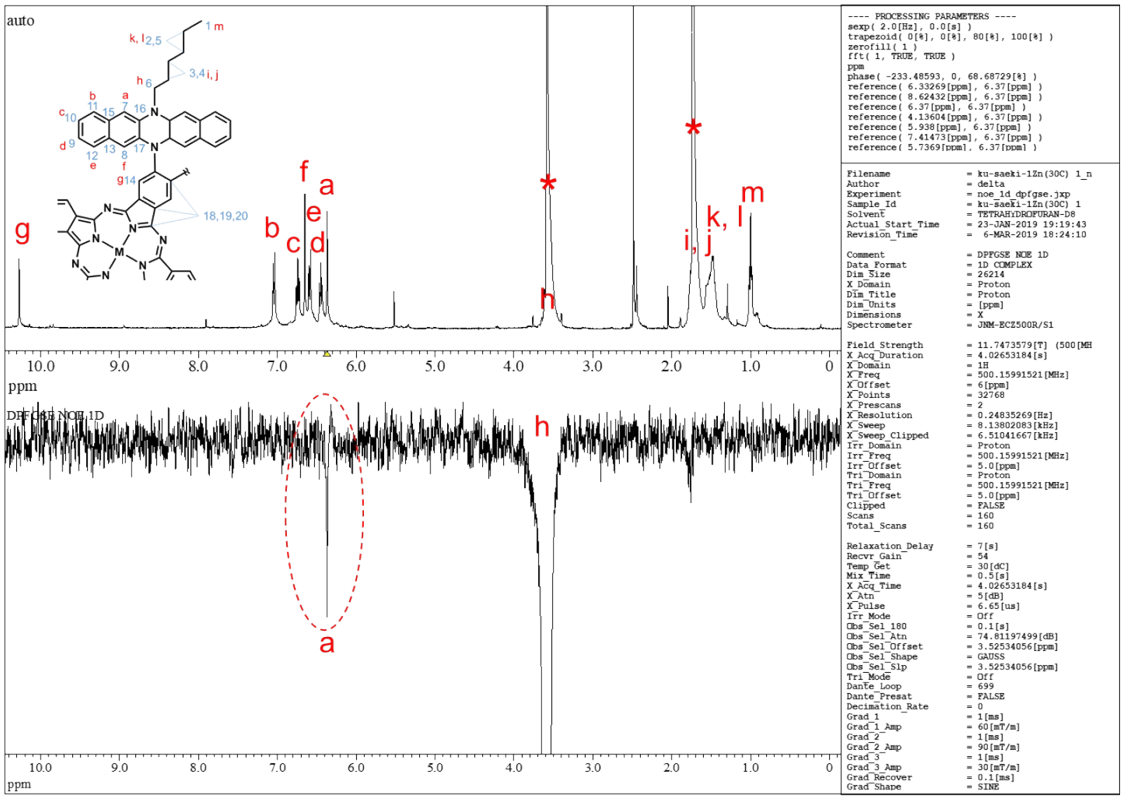

Figure S10. 1D DPFGSE-NOE spectrum of **1Zn** at 303 K. DPFGSE selective irradiation of proton h (tetrahydrofuran-d_8, 500 MHz). Mixing time was 0.5 s.

Table S1. Longitudinal relaxation time (T_1) of protons in **1Zn** estimated by double pulse measurement (tetrahydrofuran-d_8, 500 MHz).

	a	b	c	d	e	f	g	h
T_1 / s	0.85	1.71	2.00	1.90	1.80	1.88	2.37	0.56

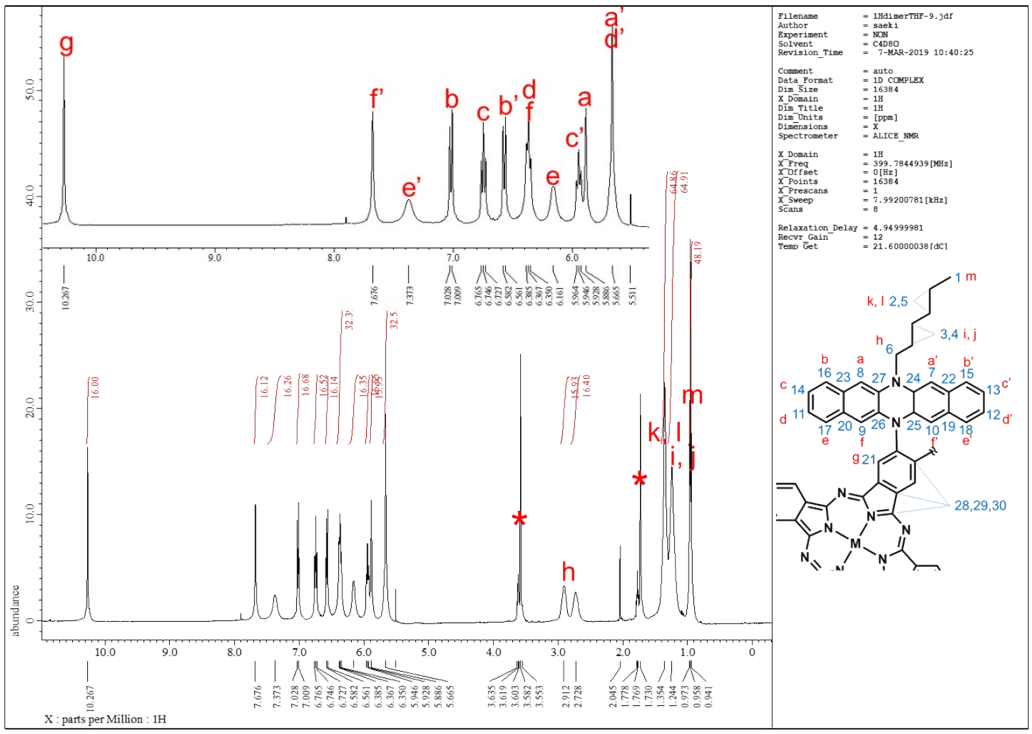

Figure S11. ^{1}H NMR spectra of **1Zn2** at 298 K (tetrahydrofuran-d_8, 400 MHz).

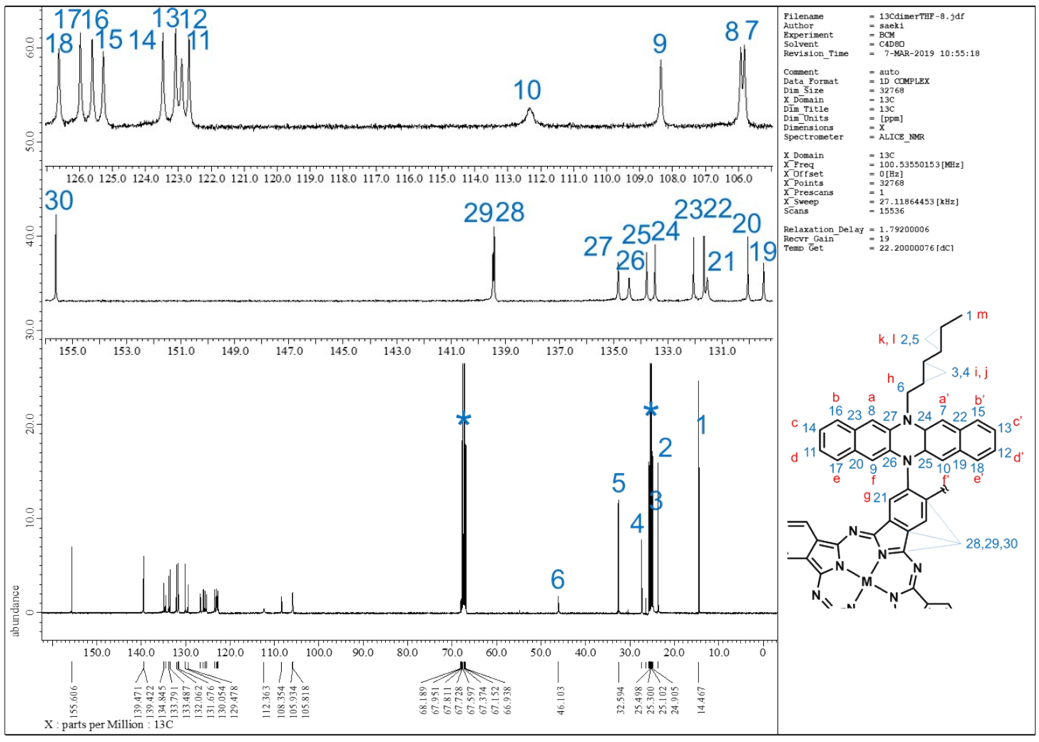

Figure S12. ^{13}C NMR spectra of **1Zn2** at 303 K (tetrahydrofran-d_8, 100 MHz).

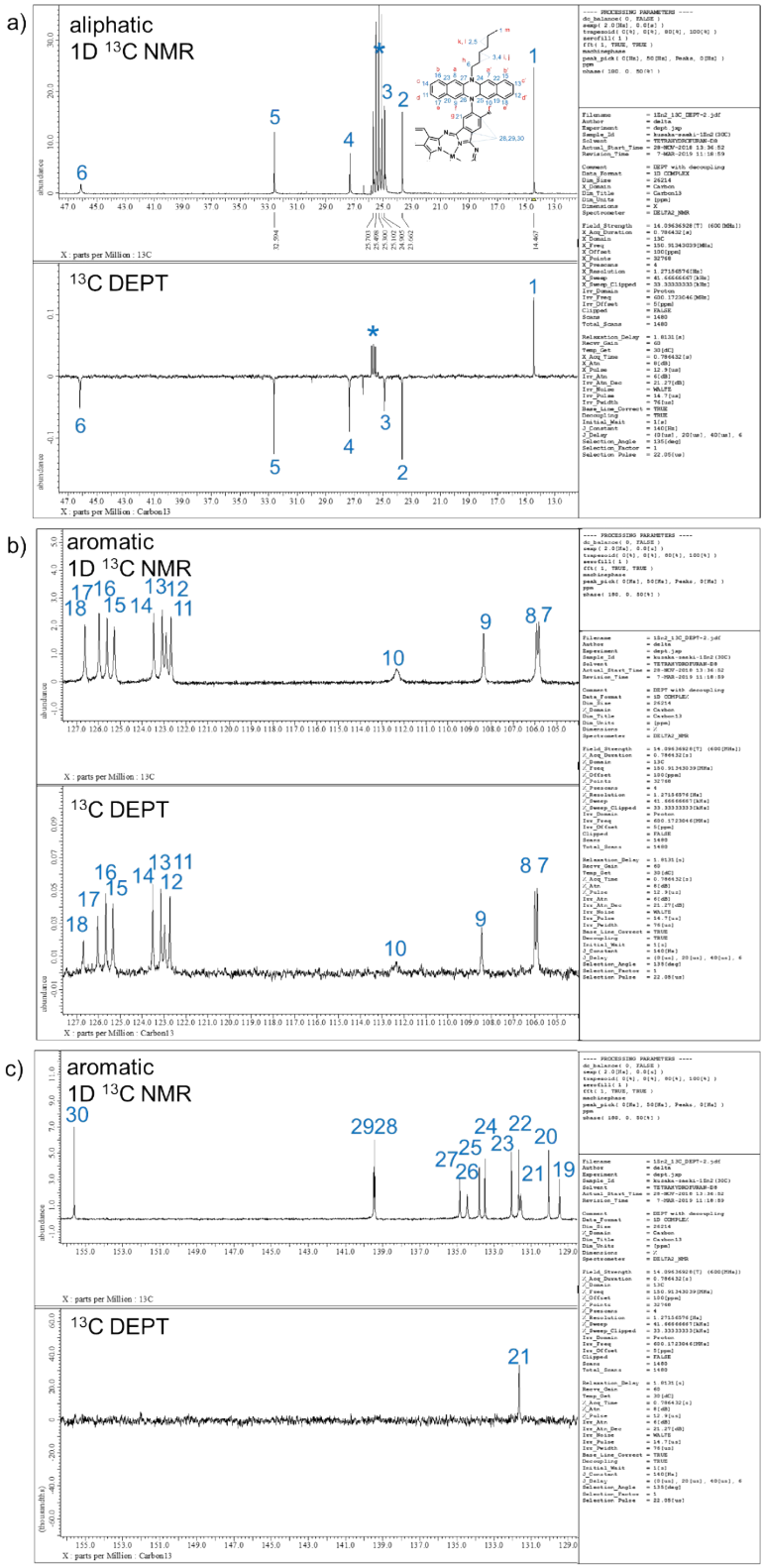

Figure S13. ^{13}C NMR and DEPT spectra of **1Zn2** at 303 K. (a) aliphatic region and (b), (c) aromatic region (tetrahydrofran-d_8, 600 MHz).

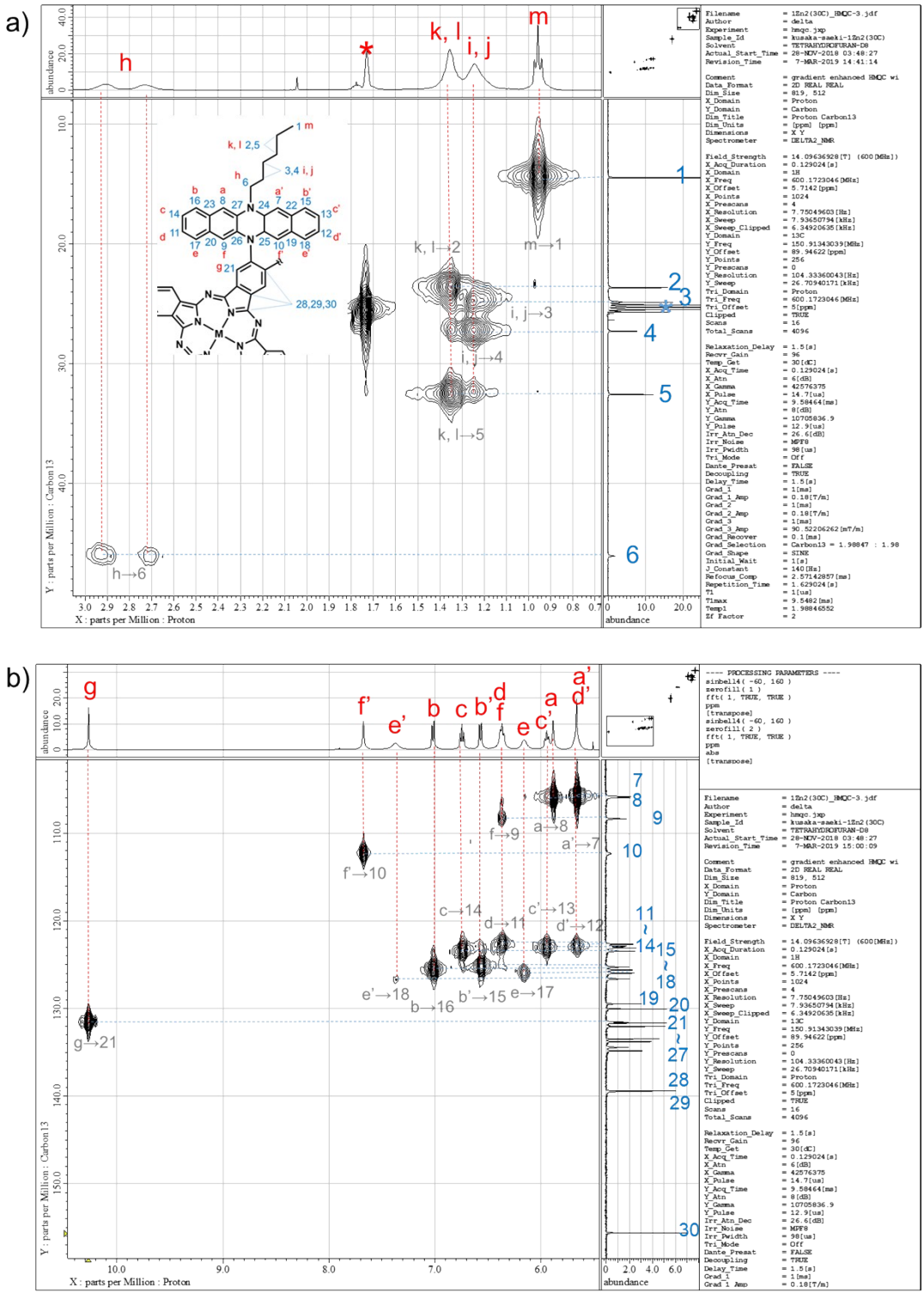

Figure S14. $^{13}C/^{1}H$ HMQC spectra of **1Zn2** at 303 K. (a) aliphatic region and (b) aromatic region (tetrahydrofuran-d_8, 600 MHz). The split of the h proton is due to the slow rotation of the C6—N bonds.

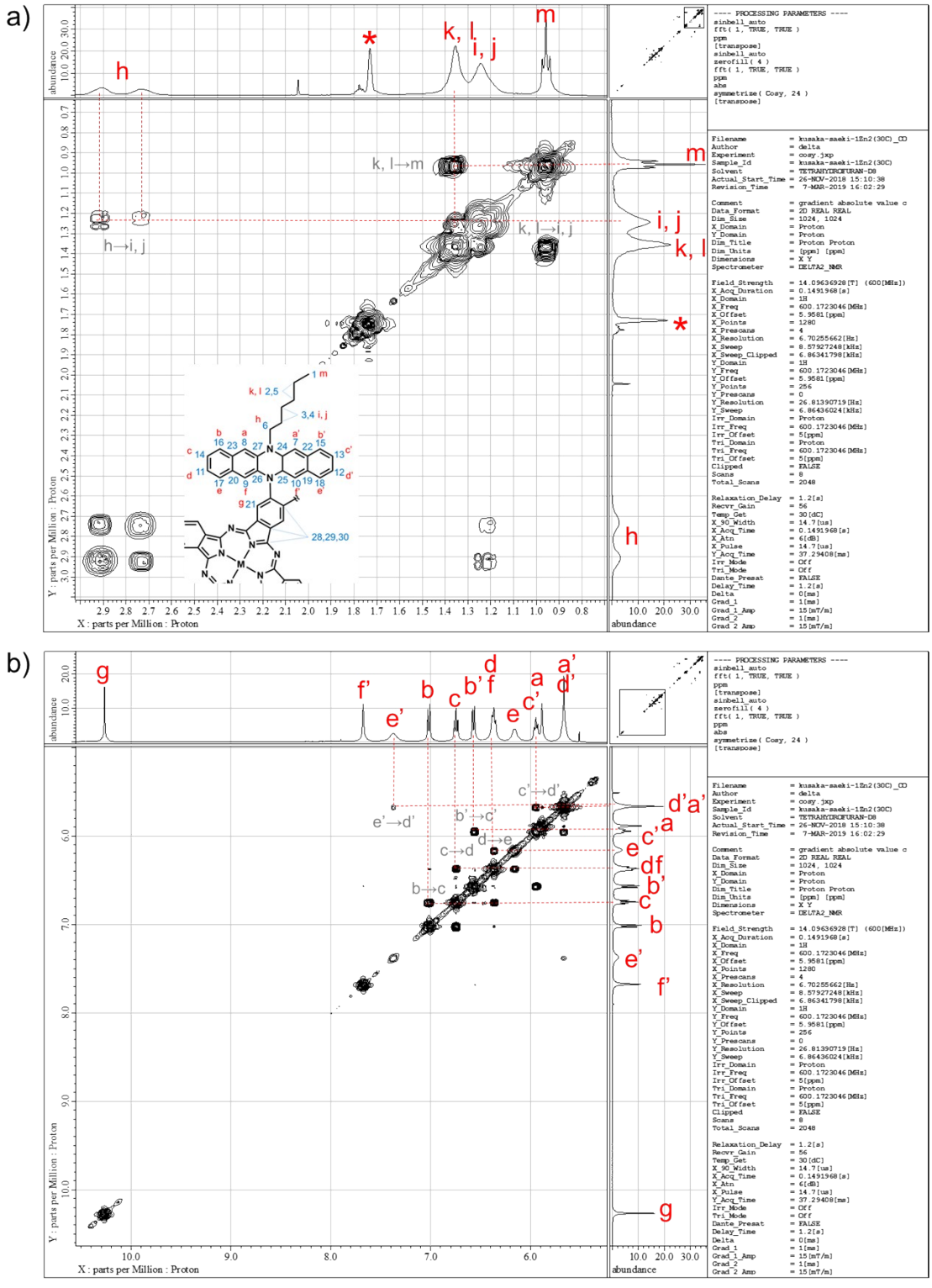

Figure S15. ^{1}H–^{1}H COSY spectra of **1Zn2** at 303 K. (a) aliphatic region and (b) aromatic region (tetrahydrofuran-d_8, 600 MHz).

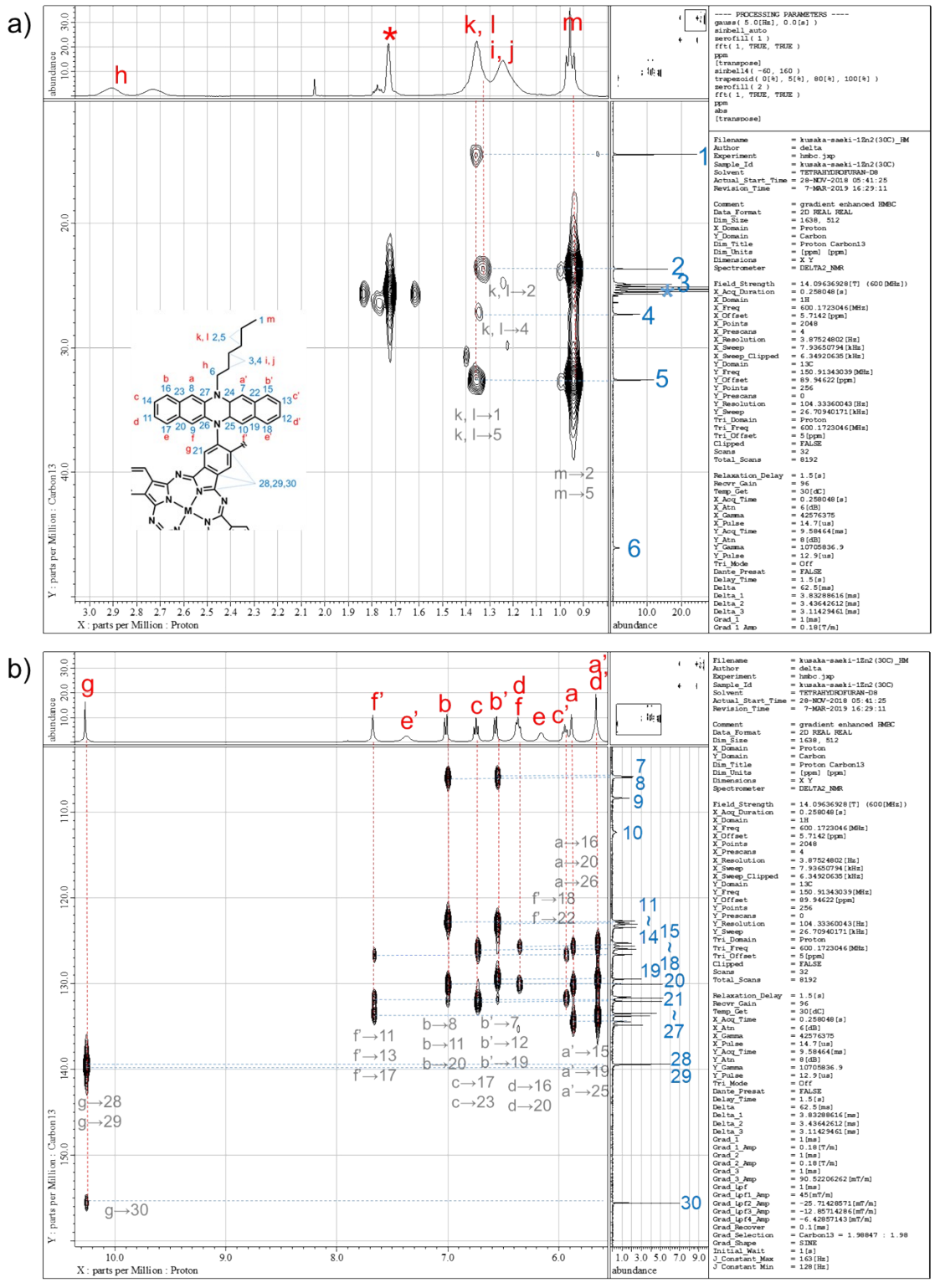

Figure S16. $^{13}C/^{1}H$ HMBC spectra of **1Zn2** at 303 K. (a) aliphatic region and (b) aromatic region (tetrahydrofuran-d_8, 600 MHz).

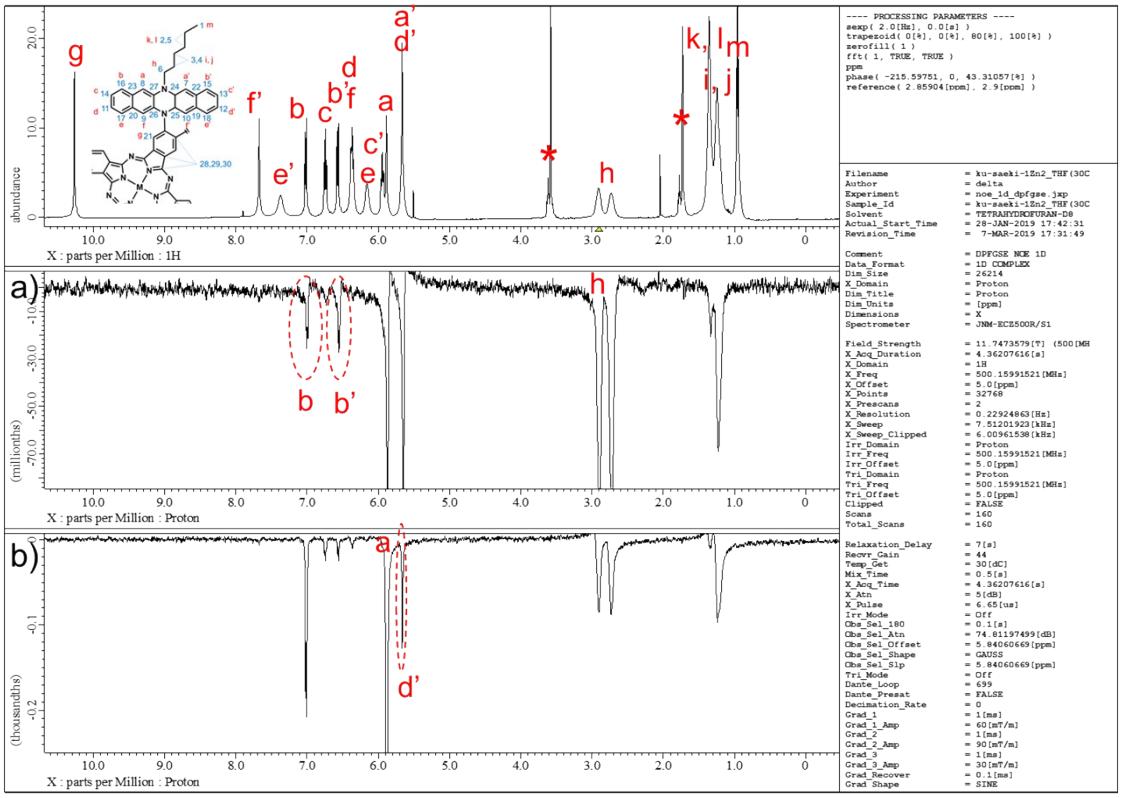

Figure S17. 1D DPFGSE-NOE spectrum of **1Zn2** at 303 K. DPFGSE selective irradiation of (a) proton h and (b) proton a (tetrahydrofuran-d_8, 500 MHz). Mixing time was 0.5 s.

Table S2. Longitudinal relaxation time (T_1) of protons in **1Zn2** estimated by double pulse measurement (tetrahydrofuran-d_8, 500 MHz).

	a (a')	b (b')	c (c')	d (d')	e (e')	f (f')	g	h
T_1 / s	1.14 (1.25)	1.98 (1.79)	2.35 (2.15)	2.38 (1.25)	2.37 (2.27)	2.38 (2.29)	2.31	0.83

NMR simulations

The NMR simulations were performed for **1Zn'** and **1Zn'2** using the Gauge Independent Atomic Orbitals (GIAO) method (Table S3). The calculated chemical shifts of the d' and f' protons of **1Zn2** were 4.62 and 8.29 ppm respectively, whereas the d and f protons of **1Zn** were 6.24 and 6.31 ppm respectively. Although the degrees of the shifts were slightly overestimated due to neglecting the molecular fluctuation, the observed shifts of these protons were qualitatively reproduced.

Table S3. Calculated ^{1}H NMR chemical shifts of **1Zn'** and **1Zn'2** (M06-2X/6-31G*, LANL2DZ).

	a (a')	b (b')	c (c')	d (d')	e (e')	f (f')	g
1Zn'	6.71	7.63	7.04	6.24	6.39	6.31	11.51
1Zn'2	5.19 (6.34)	6.89 (7.32)	7.09 (6.58)	6.77 (4.62)	6.67 (6.29)	6.00 (8.29)	11.30

^{1}H-DPFGSE-NOE for 1Zn2

Figure S18 shows a ^{1}H-DPFGSE-NOE spectrum when the protons of the benzo moieties of Pc (g) were selectively irradiated. Besides the strong peaks of f and f', which are obviously in close proximity to the g protons, the intensity of the e' proton apparently increased, whereas the intensity of the e proton was much smaller. According to the optimized geometry of **1Zn'2**, the distance between the protons of g and e' belonging to different monomers were calculated to be only 2.95 Å, whereas the distance between the protons of g and e' in a same DHDAP moiety was to be 4.47 Å, strongly indicating the proposed dimer structure.

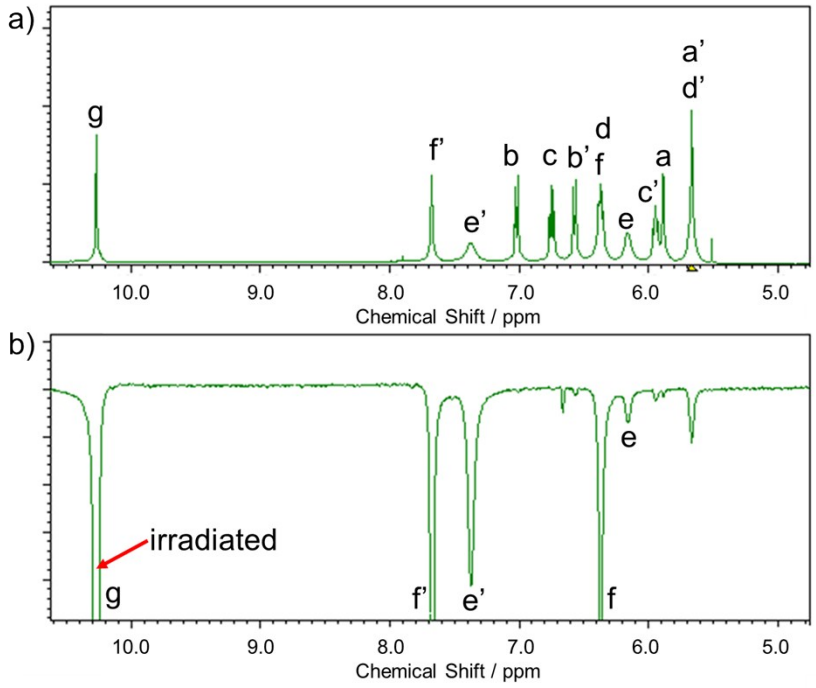

Figure S18. (a) Aromatic regions of ^{1}H NMR spectra for **1Zn2**. (b) ^{1}H-DPFGSE-NOE spectrum of **1Zn2** at 303 K (selective irradiation of the g proton).

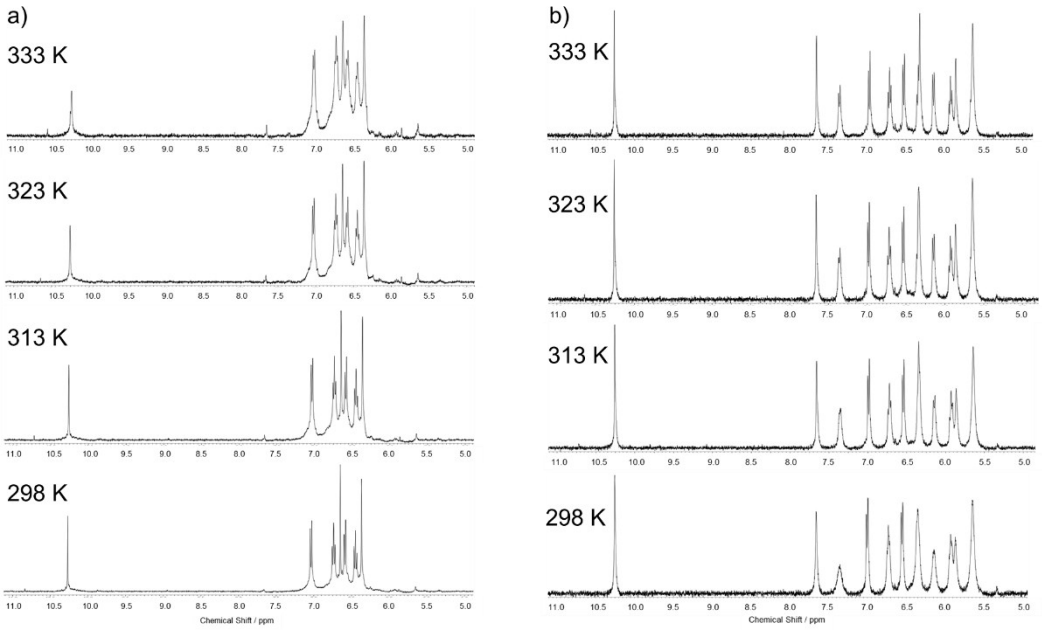

Figure S19. Variable-temperature 1H NMR spectra of a) **1Zn** and b) **1Zn2** in tetrahydrofuran-d_8.

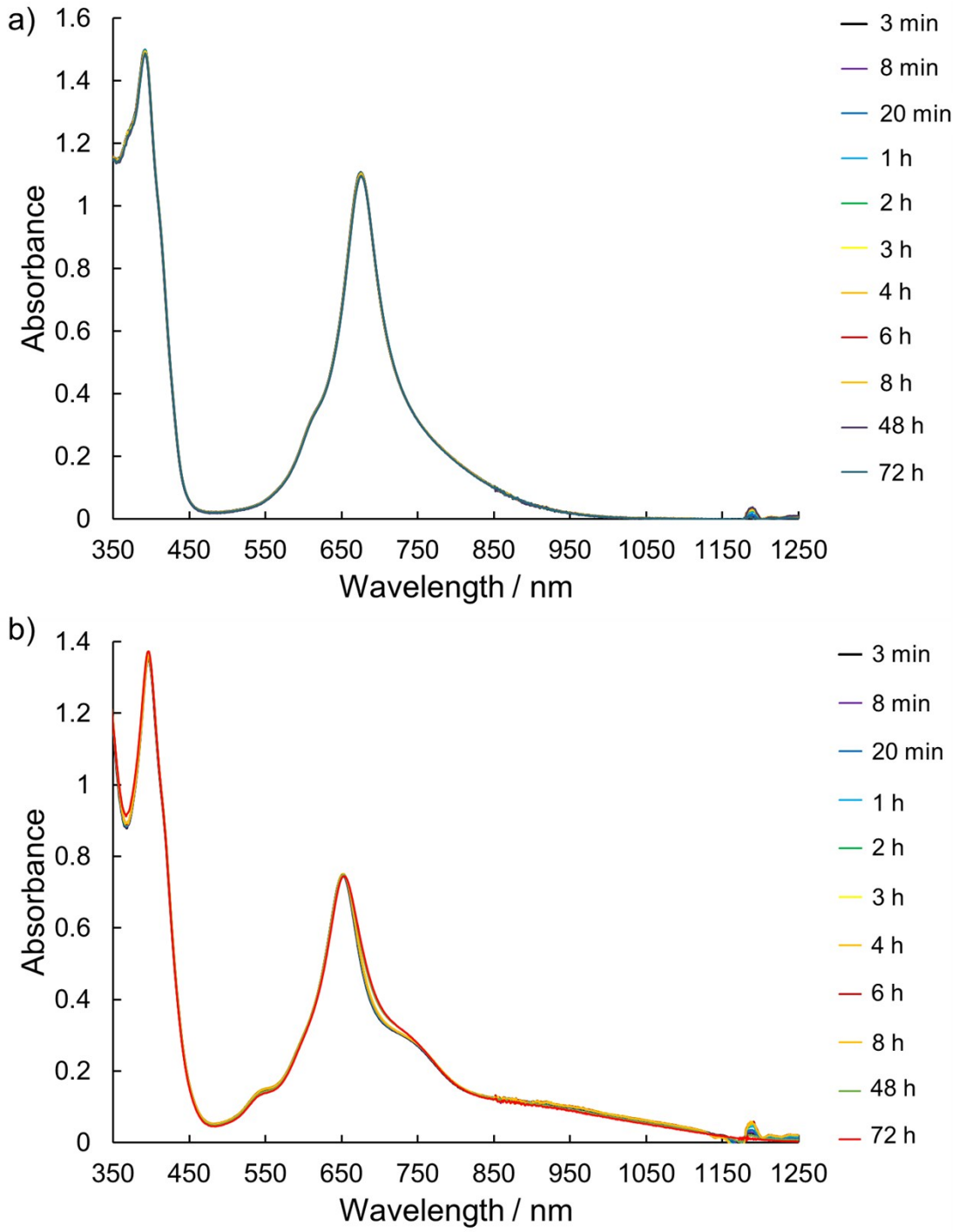

Figure S20. Temporal changes of the UV-Vis-NIR absorption spectra of (a) **1Zn** (1×10^{-5} M) and (b) **1Zn2** (5×10^{-6} M) in tetrahydrofuran at r.t.

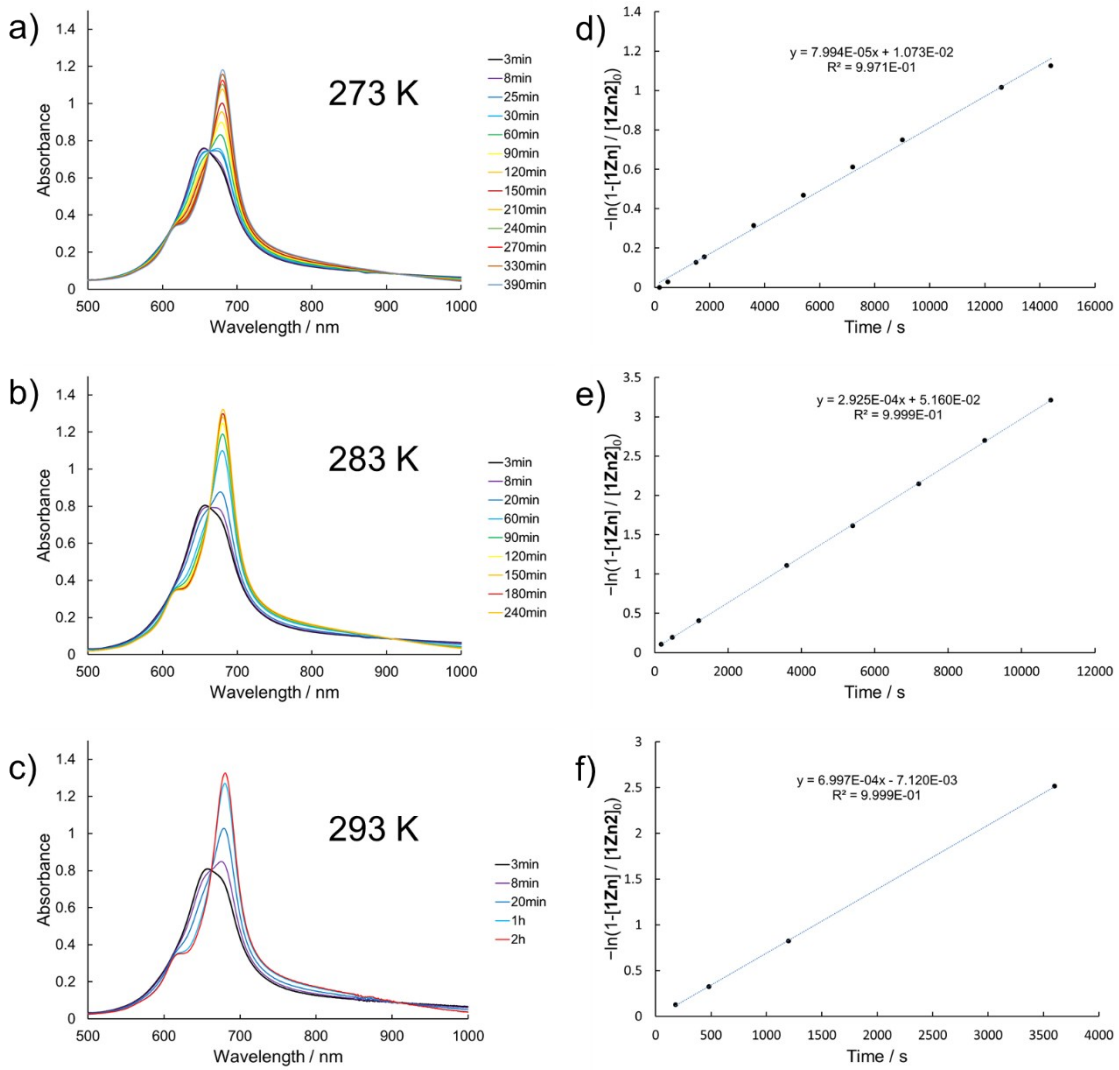

Figure S21. Temporal changes of the UV-Vis-NIR absorption spectra of **1Zn2** (5×10^{-6} M) in *o*-dichlorobenzene at a) 273 K, b) 283 K, and c) 293 K and the first-order decay plot of **1Zn2** at a) 273 K, b) 283 K, and c) 293 K.

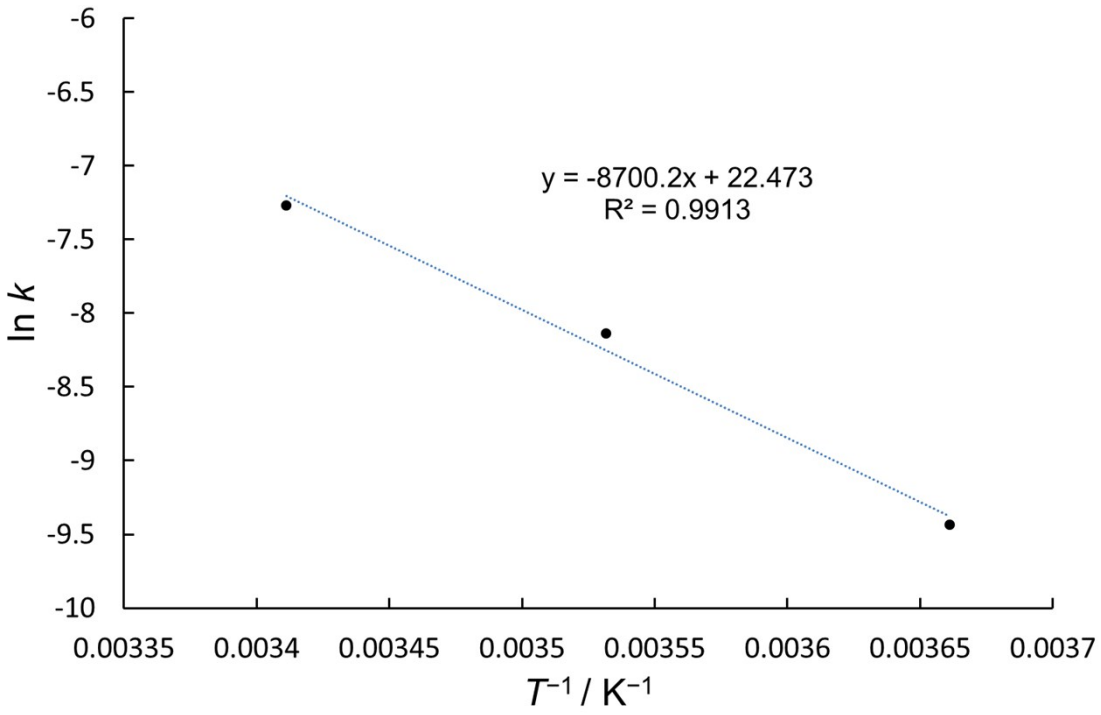

Figure S22. Arrhenius plot of the dissociation of **1Zn2** in *o*-dichlorobenzene.

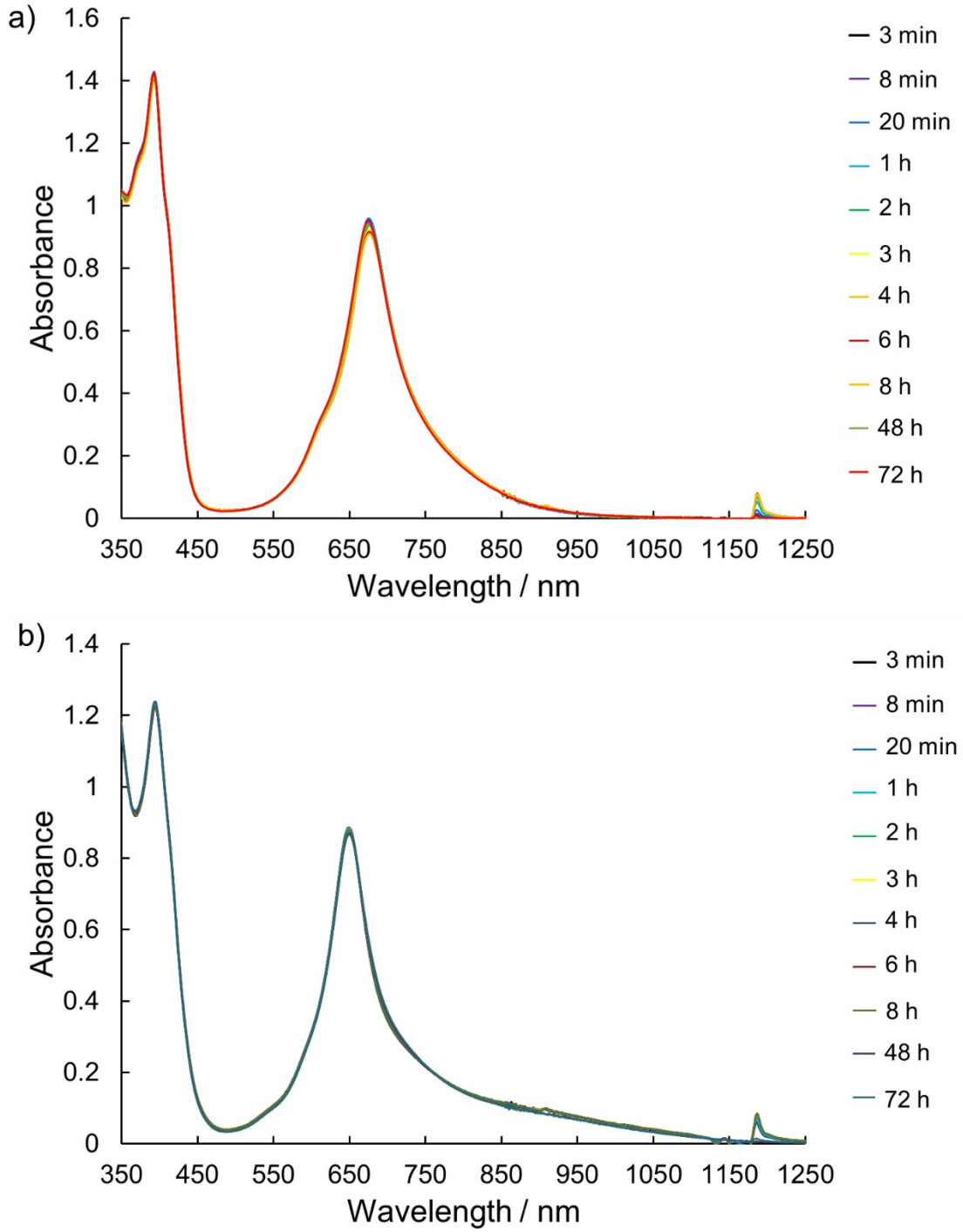

Figure S23. Temporal changes of the UV-Vis-NIR absorption spectra of (a) **1Zn** (1×10^{-5} M) and (b) **1Zn2** (5×10^{-6} M) in ethyl acetate at r.t.

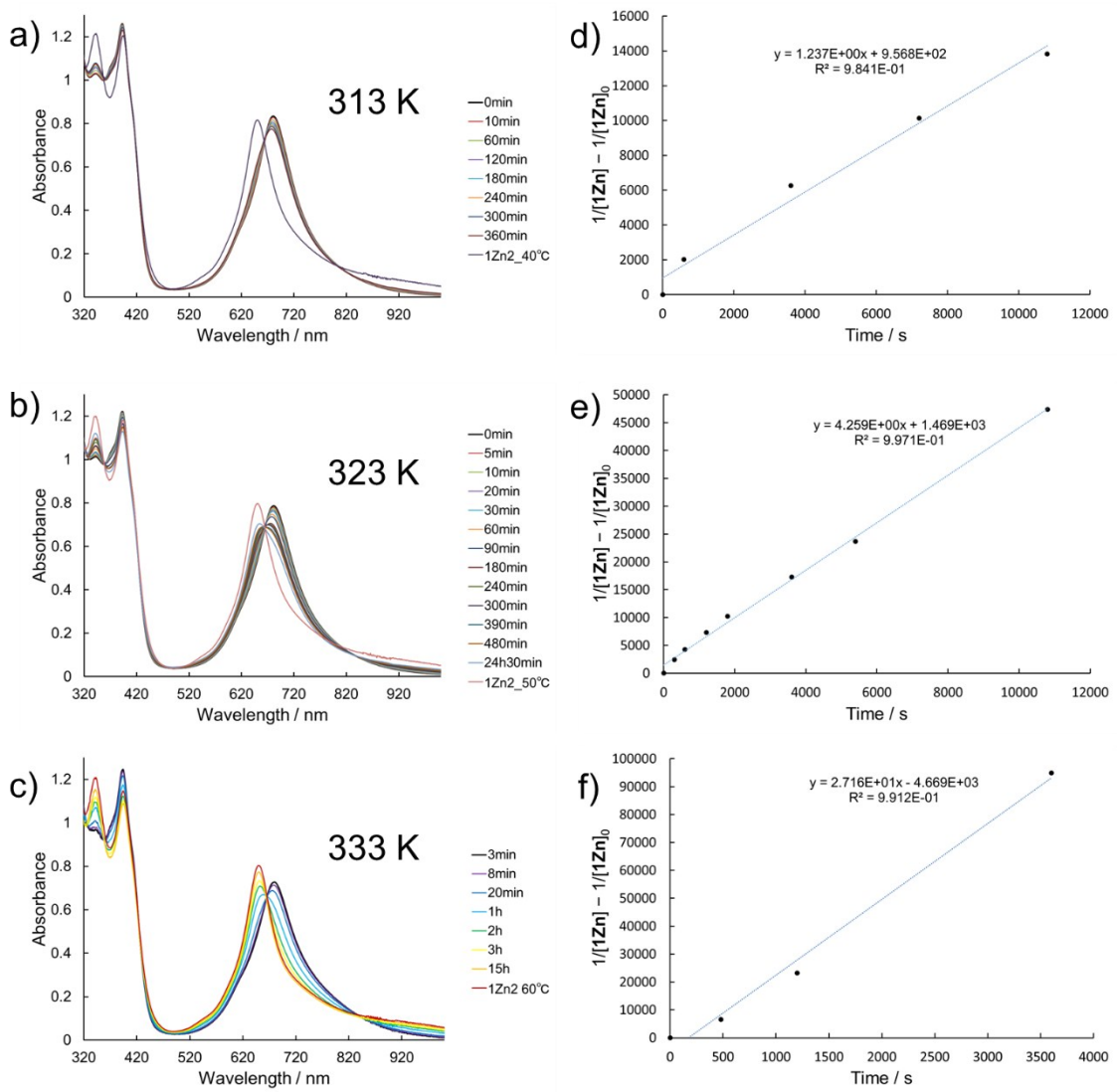

Figure S24. Temporal changes of the UV-Vis-NIR absorption spectra of **1Zn** (1×10^{-5} M) in ethyl acetate at (a) 313 K, (b) 323 K, and (c) 333 K and the second-order plot of the dimerization reaction of **1Zn** at (d) 313 K, (e) 323 K, and (c) 333 K.

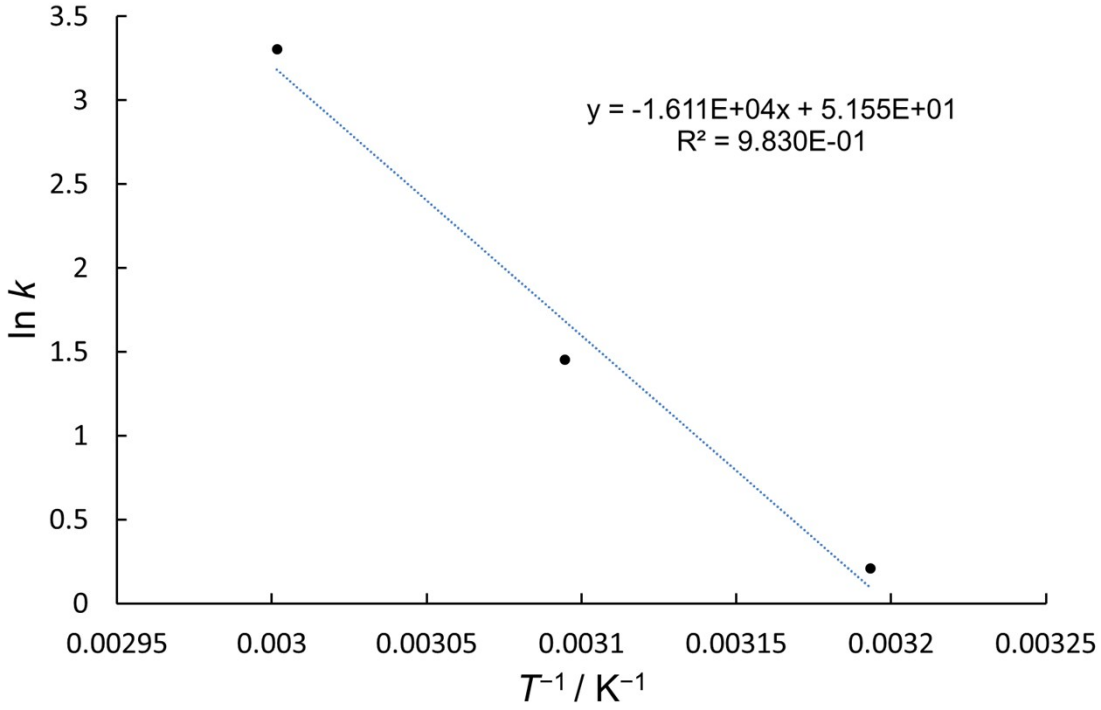

Figure S25. Arrhenius plot of the dimerization reaction of **1Zn** in ethyl acetate.

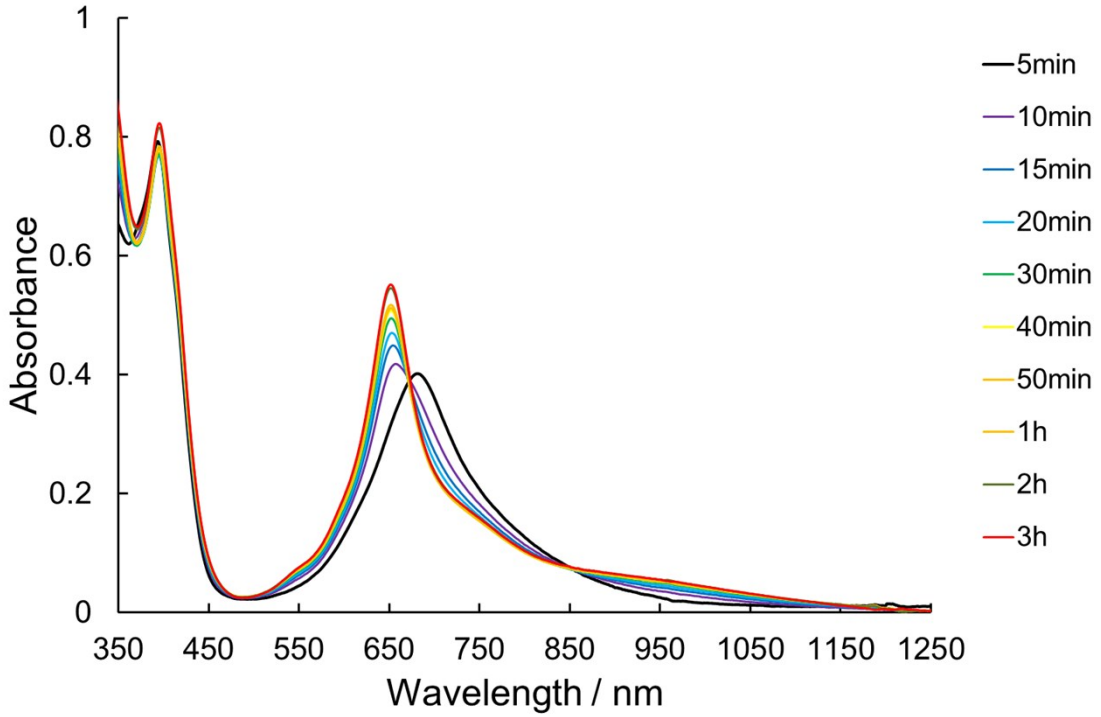

Figure S26. Temporal changes of the UV-Vis-NIR absorption spectra of **1Zn** in 1-pentanol at 373 K.

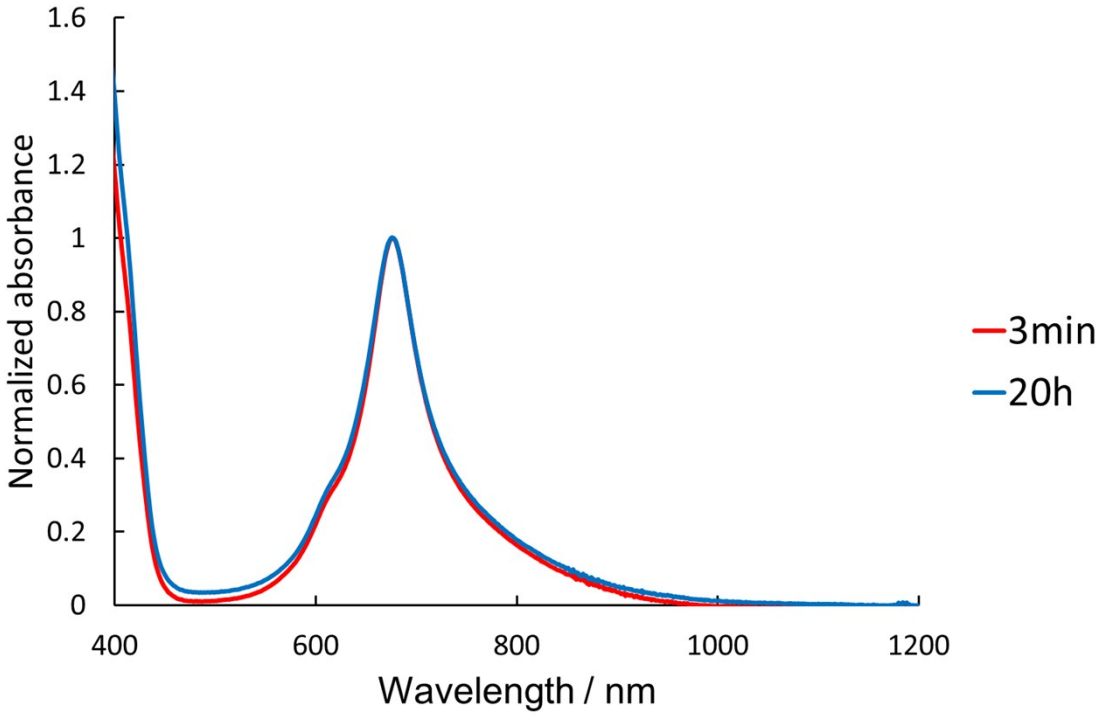

Figure S27. Temporal changes of the UV-Vis-NIR absorption spectra of **1Zn** (1×10^{-5} M) in tetrahydrofuran at 333 K.

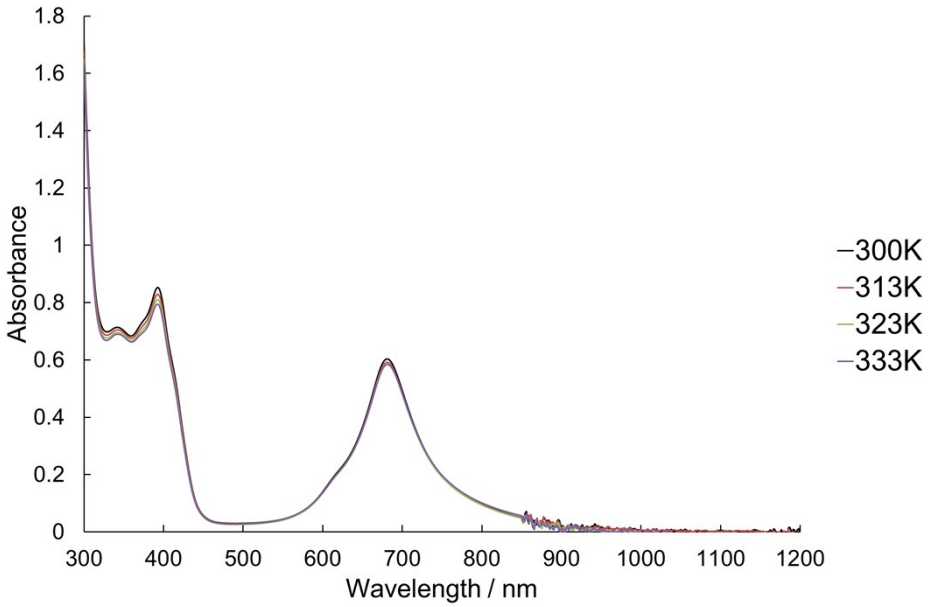

Figure S28. Variable-temperature UV-Vis-NIR absorption spectra of **1Zn** in tetrahydrofuran.

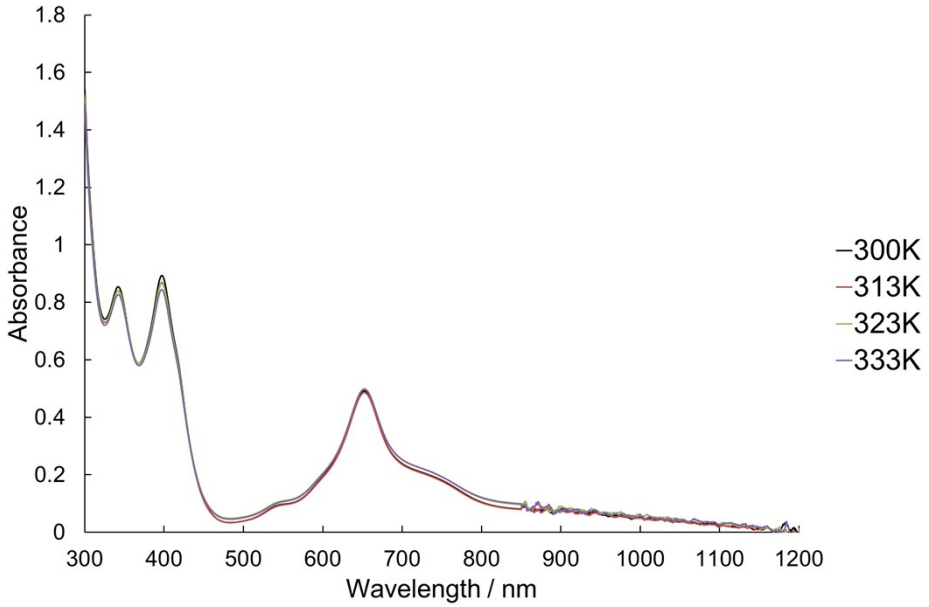

Figure S29. Variable-temperature UV-Vis-NIR absorption spectra of **1Zn2** in tetrahydrofuran.

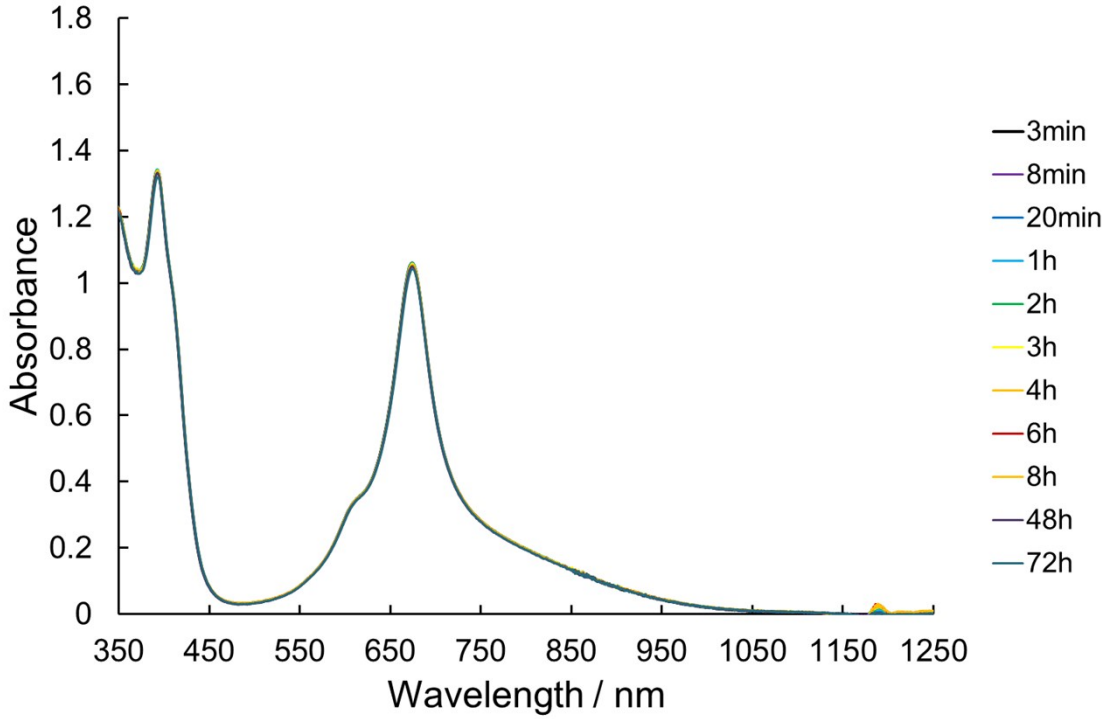

Figure S30. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu** (1×10^{-5} M) in tetrahydrofuran at r.t.

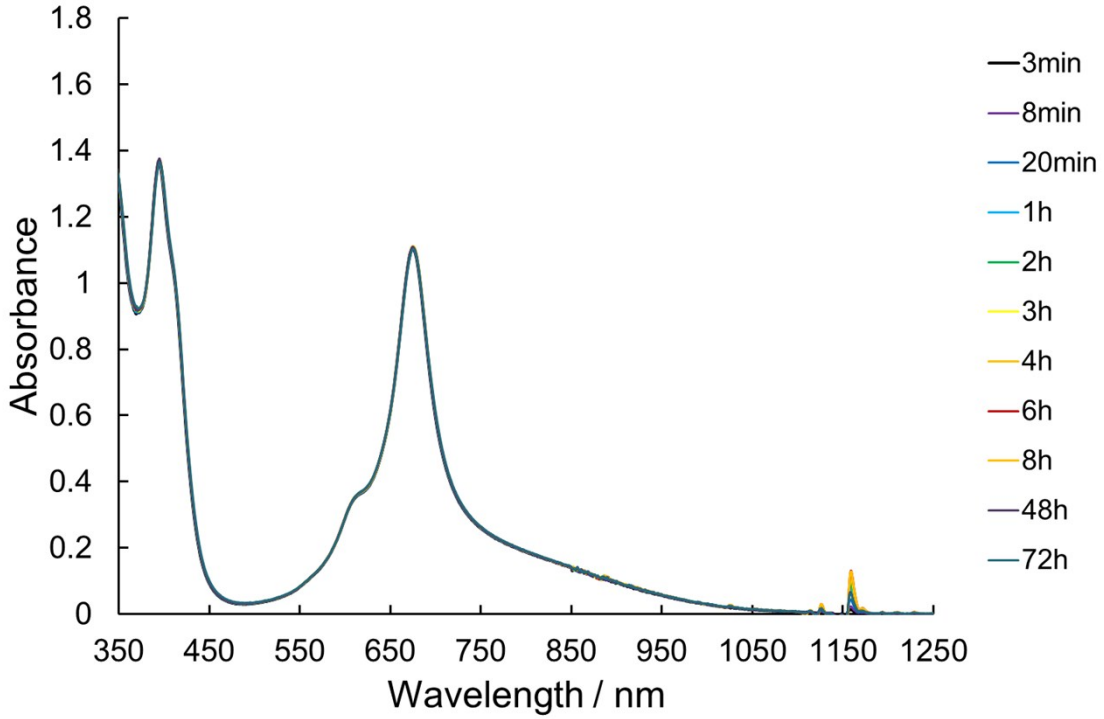

Figure S31. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu** (1×10^{-5} M) in CH_2Cl_2 at r.t.

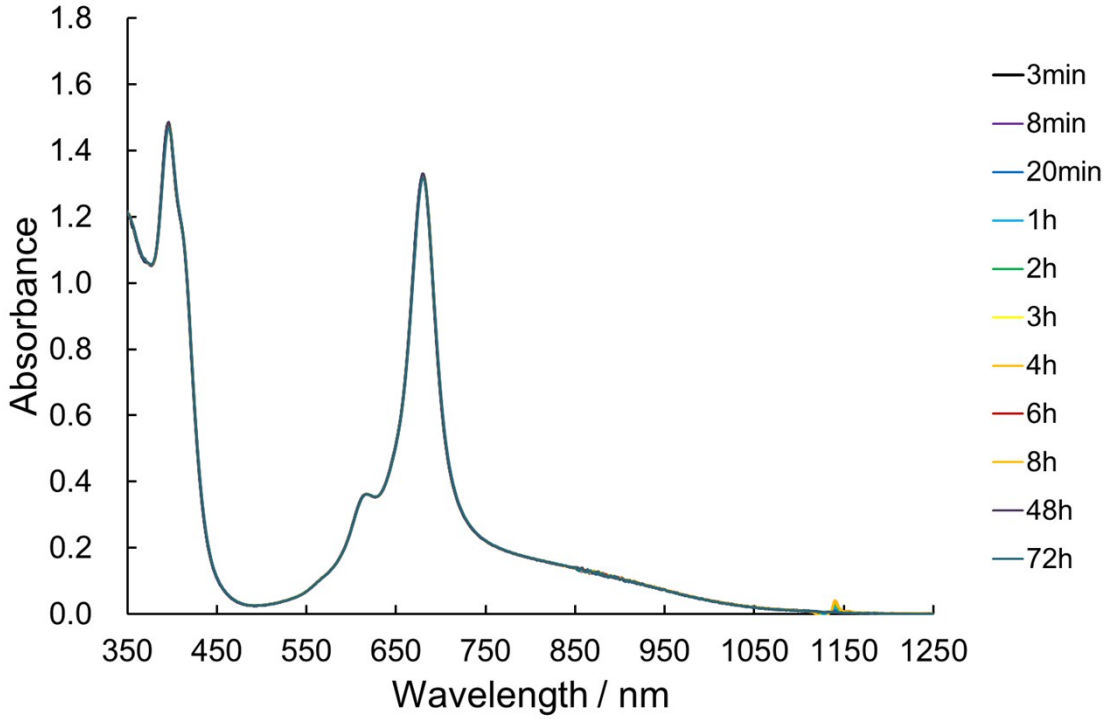

Figure S32. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu** (1×10^{-5} M) in *o*-dichlorobenzene at r.t.

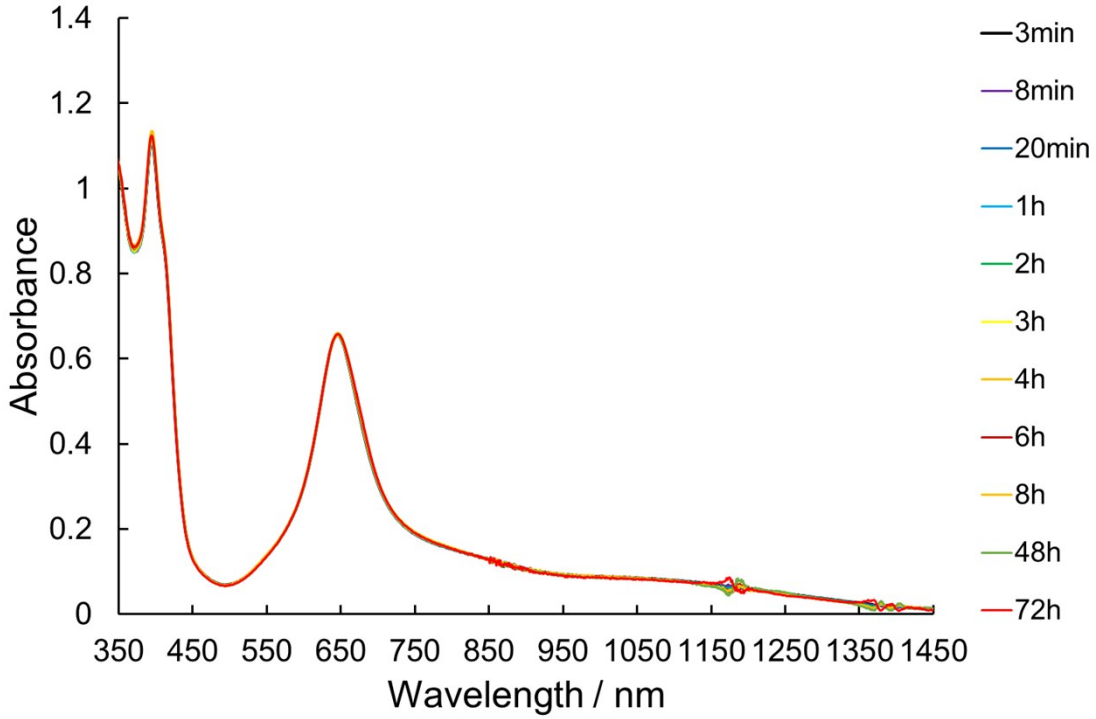

Figure S33. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu2** (5×10^{-6} M) in tetrahydrofuran at r.t.

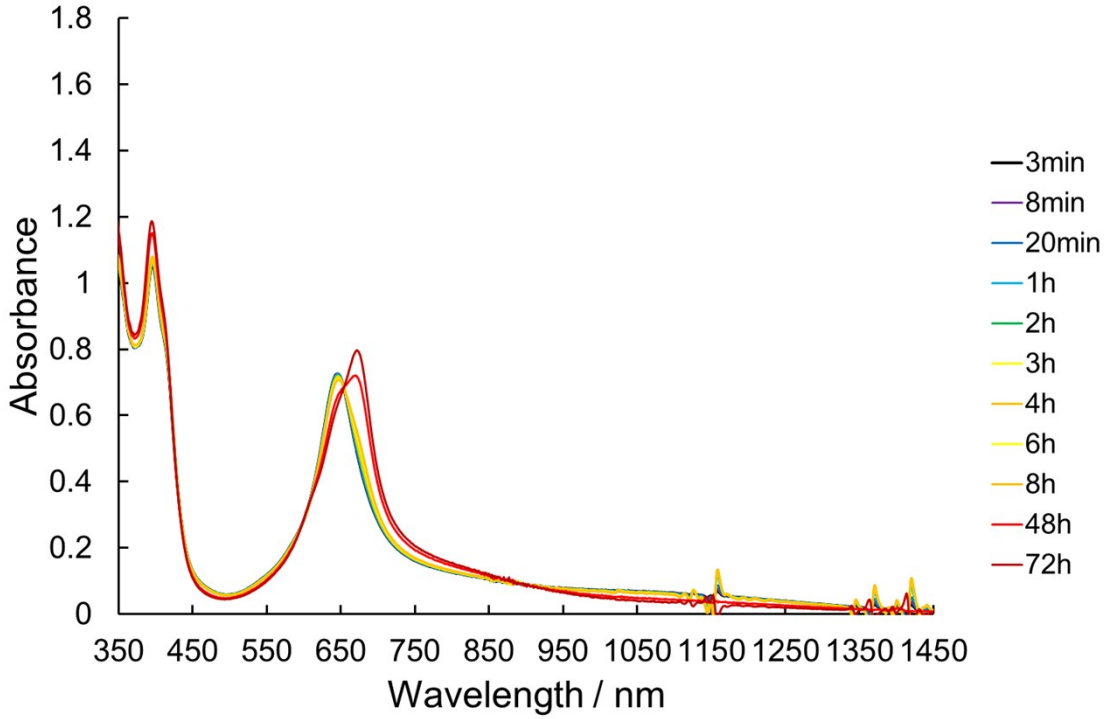

Figure S34. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu2** (5×10^{-6} M) in CH_2Cl_2 at r.t.

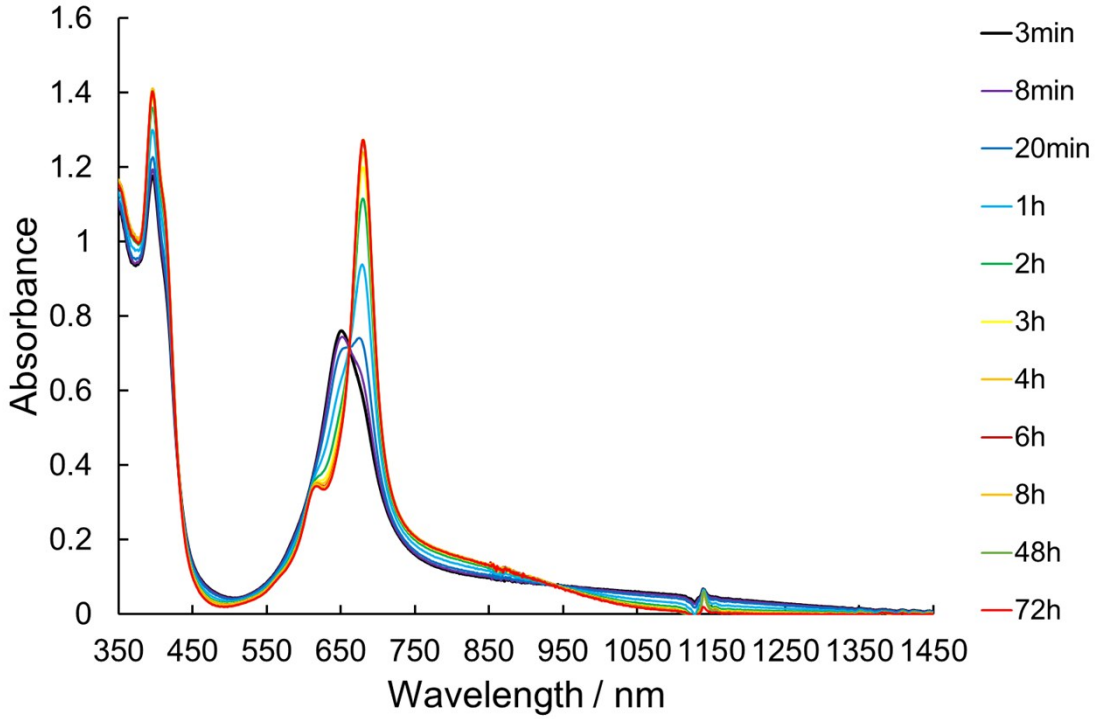

Figure S35. Temporal changes of the UV-Vis-NIR absorption spectra of **1Cu2** (5×10^{-6} M) in *o*-dichlorobenzene at r.t.

DFT calculations

To examine whether such dimers can be reasonably formed, we performed the structural optimization of the model compounds of **1Zn** and its dimer **1Zn2** in which the *n*-hexyl groups are replaced with hydrogen atoms (**1Zn'** and **1Zn'2**) for the ease of calculations using density functional theory (DFT). We have used the M06-2X functional for the calculations, which could well reproduce the crystal structure of **2** with the co-facially stacked DHDAP units similar to our previous report. The optimized structure of **1Zn'** has D_4 symmetry, and the four pairs of the co-facially stacked DHDAP units are slightly tilted by ~18° respect to the Pc plane (Figure S36a). As can be seen from the top view, **1Zn'** has four large voids between each pair of DHDAP units, which can accommodate the DHDAP pairs of the other monomer. Next, we have carried out the structural optimization of **1Zn'2** with the structure in which two **1Zn'** interdigitated. Figure S32b shows the optimized geometry of **1Zn'2**. As expected, two **1Zn'** molecules are closely bound to each other filling each other's voids with DHDAP units, and about three of five six-membered rings of each DHDAP unit are inserted into the voids of the other monomer. The small distance between two Zn atoms (3.315 Å) suggests the existence of the strong attractive interaction between two **1Zn'** molecules.

Besides the π–π stacking between two Pc planes, there are some intermonomer short contacts (< 3.4 Å) between DHDAP units belonging to different monomers, indicating the intermonomer π–π interactions among the pillar-like peripheral substituents. For example, the shortest intermonomer N···C distances for each nitrogen atoms in the DHDAP moieties are shown in Figure S36c.

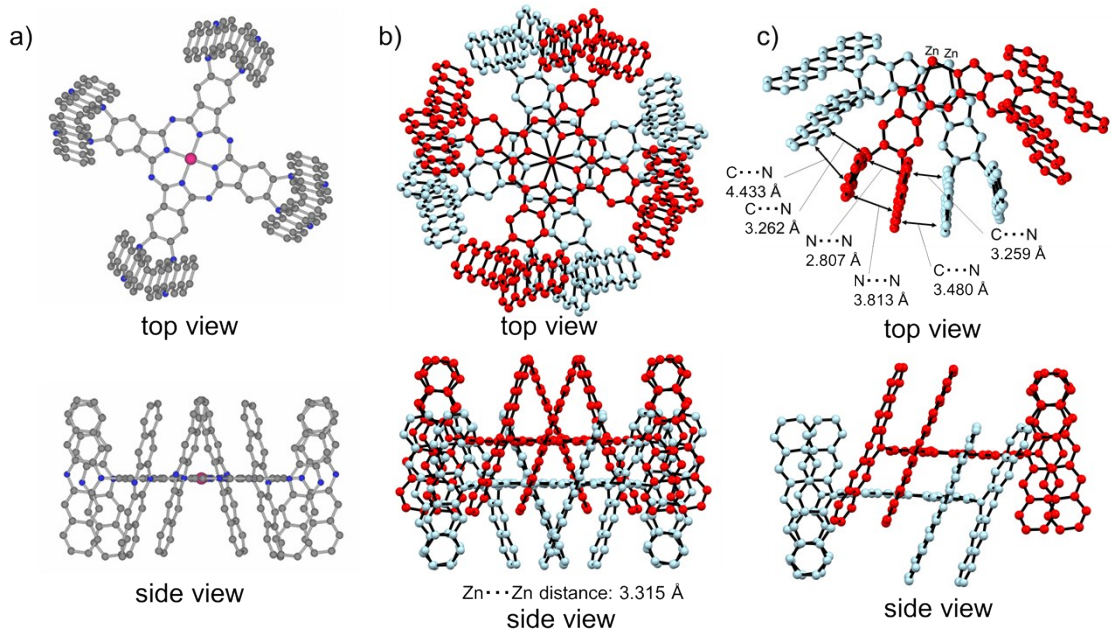

Figure S36. Optimized structures of a) **1Zn'** and b) **1Zn'2** (each monomer is shown in a different color) calculated at the M06-2X/6-31G(d) (for H, C, N), LANL2DZ (for Zn) level of theory. c) Partial structure of **1Zn'2**.

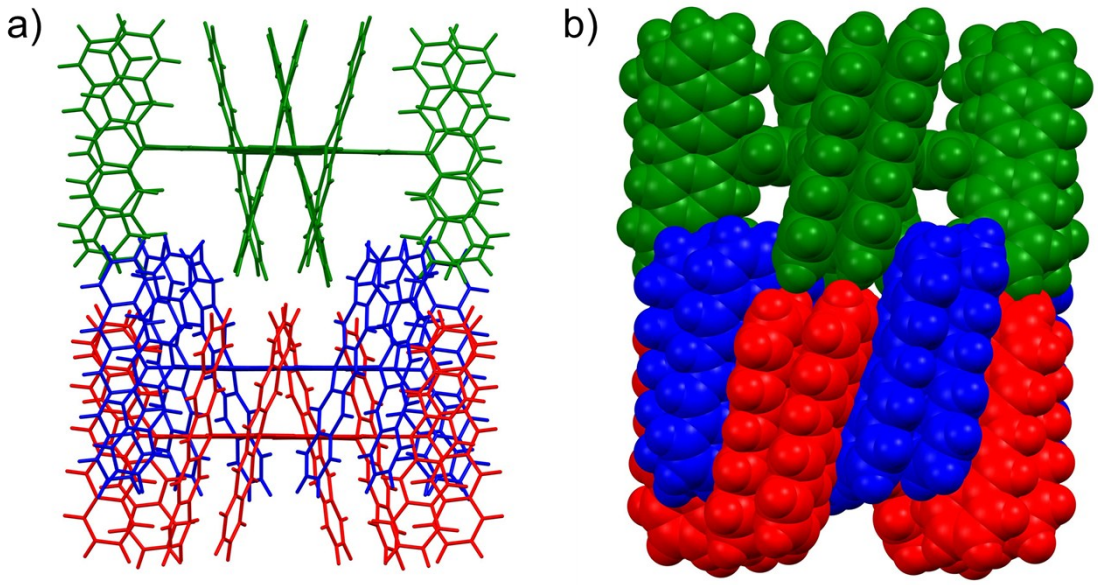

Figure S37. Molecular model of **1Zn'3** (each monomer is shown in a different color) shown in a) wireframe model and b) space filling model.

1Zn' (D_4) M06-2X/6-31G* (for C, H, and N) LANL2DZ (for Zn)
E = −8760.41784319 hartree

C	−1.119984	2.785701	0.000495
C	−0.700881	4.187260	0.002415
N	−1.412232	7.814289	0.029880
C	0.700881	4.187260	−0.002415
N	1.412232	7.814289	−0.029880
C	1.119984	2.785701	−0.000495
N	−2.387666	2.387666	0.000000
N	0.000000	2.007877	0.000000
C	1.900515	8.312210	−1.258831
C	1.304802	8.642260	1.109110
C	1.438218	10.057298	0.948560
C	2.011064	9.733677	−1.408556
N	1.722848	10.538053	−0.316384

C	1.259670	10.889646	2.026120
C	2.371141	10.271183	−2.617728
H	1.804020	11.536621	−0.437867
C	−1.900515	8.312210	1.258831
C	−1.304802	8.642260	−1.109110
C	−1.438218	10.057298	−0.948560
C	−2.011064	9.733677	1.408556
N	−1.722848	10.538053	0.316384
C	−1.259670	10.889646	−2.026120
C	−2.371141	10.271183	2.617728
H	−1.804020	11.536621	0.437867
C	0.929209	10.379133	3.307434
H	1.351933	11.965449	1.889769
C	0.681806	11.220606	4.420908
C	0.824434	8.972737	3.474868
C	1.042523	8.129542	2.353027
H	0.950086	7.054926	2.482728
C	0.348018	10.687712	5.642533
H	0.759261	12.297441	4.290620
H	0.152204	11.343923	6.485397
C	0.249502	9.287610	5.809929
C	0.484986	8.451100	4.746719
H	−0.033723	8.877283	6.773831
H	0.390060	7.374034	4.861076
C	2.644963	9.452147	−3.741425
H	2.416260	11.352711	−2.727892
C	2.984956	9.990533	−5.005491
C	2.564413	8.043152	−3.589261
C	2.193656	7.504362	−2.327582
H	2.099993	6.427314	−2.236614
C	3.231363	9.165751	−6.076371
H	3.035134	11.070785	−5.116429
H	3.487648	9.590125	−7.042383
C	3.149928	7.762917	−5.927024
C	2.825046	7.215834	−4.708621
H	3.349507	7.118110	−6.777375

H	2.761739	6.137103	−4.587041
C	−0.929209	10.379133	−3.307434
H	−1.351933	11.965449	−1.889769
C	−0.824434	8.972737	−3.474868
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H	−2.416260	11.352711	2.727892
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C	−2.825046	7.215834	4.708621
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C	−0.249502	9.287610	−5.809929
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H	−0.759261	12.297441	−4.290620
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C	−2.984956	9.990533	5.005491
H	−3.487648	9.590125	7.042383
H	−3.035134	11.070785	5.116429
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H	2.506820	5.388464	0.008970
C	−0.714573	6.575620	0.009225
C	−1.421204	5.379283	0.003713
H	−2.506820	5.388464	−0.008970
C	2.785701	1.119984	0.000495
C	4.187260	0.700881	0.002415
N	7.814289	1.412232	0.029880

C	4.187260	−0.700881	−0.002415
N	7.814289	−1.412232	−0.029880
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N	2.387666	2.387666	0.000000
N	2.007877	0.000000	0.000000
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C	8.642260	−1.304802	1.109110
C	10.057298	−1.438218	0.948560
C	9.733677	−2.011064	−1.408556
N	10.538053	−1.722848	−0.316384
C	10.889646	−1.259670	2.026120
C	10.271183	−2.371141	−2.617728
H	11.536621	−1.804020	−0.437867
C	8.312210	1.900515	1.258831
C	8.642260	1.304802	−1.109110
C	10.057298	1.438218	−0.948560
C	9.733677	2.011064	1.408556
N	10.538053	1.722848	0.316384
C	10.889646	1.259670	−2.026120
C	10.271183	2.371141	2.617728
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C	8.451100	−0.484986	4.746719
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H	11.352711	−2.416260	−2.727892

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H	9.590125	−3.487648	−7.042383
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C	8.451100	0.484986	−4.746719
H	7.054926	0.950086	−2.482728
C	9.452147	2.644963	3.741425
H	11.352711	2.416260	2.727892
C	8.043152	2.564413	3.589261
C	7.504362	2.193656	2.327582
C	7.215834	2.825046	4.708621
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H	7.374034	0.390060	−4.861076
H	8.877283	−0.033723	−6.773831
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C	11.220606	0.681806	−4.420908
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H	12.297441	0.759261	−4.290620
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H	6.137103	2.761739	4.587041
H	7.118110	3.349507	6.777375
C	9.165751	3.231363	6.076371
C	9.990533	2.984956	5.005491
H	9.590125	3.487648	7.042383

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C	1.304802	−8.642260	−1.109110
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N	1.722848	−10.538050	0.316384
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C	−1.042523	−8.129542	2.353027

H	−0.950086	−7.054926	2.482728
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H	−0.152204	−11.343920	6.485397
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C	−0.484986	−8.451100	4.746719
H	0.033723	−8.877283	6.773831
H	−0.390060	−7.374034	4.861076
C	−2.644963	−9.452147	−3.741425
H	−2.416260	−11.352710	−2.727892
C	−2.984956	−9.990533	−5.005491
C	−2.564413	−8.043152	−3.589261
C	−2.193656	−7.504362	−2.327582
H	−2.099993	−6.427314	−2.236614
C	−3.231363	−9.165751	−6.076371
H	−3.035134	−11.070780	−5.116429
H	−3.487648	−9.590125	−7.042383
C	−3.149928	−7.762917	−5.927024
C	−2.825046	−7.215834	−4.708621
H	−3.349507	−7.118110	−6.777375
H	−2.761739	−6.137103	−4.587041
C	0.929209	−10.379130	−3.307434
H	1.351933	−11.965440	−1.889769
C	0.824434	−8.972737	−3.474868
C	1.042523	−8.129542	−2.353027
C	0.484986	−8.451100	−4.746719
H	0.950086	−7.054926	−2.482728
C	2.644963	−9.452147	3.741425
H	2.416260	−11.352710	2.727892
C	2.564413	−8.043152	3.589261
C	2.193656	−7.504362	2.327582
C	2.825046	−7.215834	4.708621
H	2.099993	−6.427314	2.236614
C	0.249502	−9.287610	−5.809929
H	0.390060	−7.374034	−4.861076
H	−0.033723	−8.877283	−6.773831

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C	0.681806	−11.220600	−4.420908
H	0.152204	−11.343920	−6.485397
H	0.759261	−12.297440	−4.290620
C	3.149928	−7.762917	5.927024
H	2.761739	−6.137103	4.587041
H	3.349507	−7.118110	6.777375
C	3.231363	−9.165751	6.076371
C	2.984956	−9.990533	5.005491
H	3.487648	−9.590125	7.042383
H	3.035134	−11.070780	5.116429
C	−1.421204	−5.379283	−0.003713
C	−0.714573	−6.575620	−0.009225
H	−2.506820	−5.388464	0.008970
C	0.714573	−6.575620	0.009225
C	1.421204	−5.379283	0.003713
H	2.506820	−5.388464	−0.008970
C	−2.785701	−1.119984	0.000495
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N	−7.814289	−1.412232	0.029880
C	−4.187260	0.700881	−0.002415
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C	−2.785701	1.119984	−0.000495
N	−2.387666	−2.387666	0.000000
N	−2.007877	0.000000	0.000000
C	−8.312210	1.900515	−1.258831
C	−8.642260	1.304802	1.109110
C	−10.057290	1.438218	0.948560
C	−9.733677	2.011064	−1.408556
N	−10.538050	1.722848	−0.316384
C	−10.889640	1.259670	2.026120
C	−10.271180	2.371141	−2.617728
H	−11.536620	1.804020	−0.437867
C	−8.312210	−1.900515	1.258831
C	−8.642260	−1.304802	−1.109110
C	−10.057290	−1.438218	−0.948560

C	−9.733677	−2.011064	1.408556
N	−10.538050	−1.722848	0.316384
C	−10.889640	−1.259670	−2.026120
C	−10.271180	−2.371141	2.617728
H	−11.536620	−1.804020	0.437867
C	−10.379130	0.929209	3.307434
H	−11.965440	1.351933	1.889769
C	−11.220600	0.681806	4.420908
C	−8.972737	0.824434	3.474868
C	−8.129542	1.042523	2.353027
H	−7.054926	0.950086	2.482728
C	−10.687710	0.348018	5.642533
H	−12.297440	0.759261	4.290620
H	−11.343920	0.152204	6.485397
C	−9.287610	0.249502	5.809929
C	−8.451100	0.484986	4.746719
H	−8.877283	−0.033723	6.773831
H	−7.374034	0.390060	4.861076
C	−9.452147	2.644963	−3.741425
H	−11.352710	2.416260	−2.727892
C	−9.990533	2.984956	−5.005491
C	−8.043152	2.564413	−3.589261
C	−7.504362	2.193656	−2.327582
H	−6.427314	2.099993	−2.236614
C	−9.165751	3.231363	−6.076371
H	−11.070780	3.035134	−5.116429
H	−9.590125	3.487648	−7.042383
C	−7.762917	3.149928	−5.927024
C	−7.215834	2.825046	−4.708621
H	−7.118110	3.349507	−6.777375
H	−6.137103	2.761739	−4.587041
C	−10.379130	−0.929209	−3.307434
H	−11.965440	−1.351933	−1.889769
C	−8.972737	−0.824434	−3.474868
C	−8.129542	−1.042523	−2.353027
C	−8.451100	−0.484986	−4.746719

H	−7.054926	−0.950086	−2.482728
C	−9.452147	−2.644963	3.741425
H	−11.352710	−2.416260	2.727892
C	−8.043152	−2.564413	3.589261
C	−7.504362	−2.193656	2.327582
C	−7.215834	−2.825046	4.708621
H	−6.427314	−2.099993	2.236614
C	−9.287610	−0.249502	−5.809929
H	−7.374034	−0.390060	−4.861076
H	−8.877283	0.033723	−6.773831
C	−10.687710	−0.348018	−5.642533
C	−11.220600	−0.681806	−4.420908
H	−11.343920	−0.152204	−6.485397
H	−12.297440	−0.759261	−4.290620
C	−7.762917	−3.149928	5.927024
H	−6.137103	−2.761739	4.587041
H	−7.118110	−3.349507	6.777375
C	−9.165751	−3.231363	6.076371
C	−9.990533	−2.984956	5.005491
H	−9.590125	−3.487648	7.042383
H	−11.070780	−3.035134	5.116429
C	−5.379283	1.421204	−0.003713
C	−6.575620	0.714573	−0.009225
H	−5.388464	2.506820	0.008970
C	−6.575620	−0.714573	0.009225
C	−5.379283	−1.421204	0.003713
H	−5.388464	−2.506820	−0.008970
Z	0.000000	0.000000	0.000000

1Zn'2 (D_4) M06-2X/6-31G* (for C, H, and N) LANL2DZ (for Zn)

E = −17520.9877471 hartree

C	1.930277	2.304499	1.570278
C	1.963658	3.767678	1.564064
N	3.732438	7.014457	1.837075

C	0.630413	4.196701	1.589538
N	1.054370	7.855320	1.858820
C	−0.201784	2.994672	1.582425
N	3.011094	1.531417	1.579821
N	0.623187	1.907832	1.577230
C	0.528050	8.313663	3.086447
C	1.433585	8.747724	0.832706
C	1.384734	10.155404	1.084693
C	0.505671	9.727680	3.323311
N	0.966108	10.580202	2.331285
C	1.761565	11.044033	0.107395
C	0.067693	10.220006	4.525266
H	0.756285	11.561769	2.441618
C	4.480163	7.504964	0.741638
C	3.740728	7.693725	3.076344
C	4.136632	9.068869	3.101869
C	4.960129	8.853077	0.815837
N	4.631666	9.609114	1.931171
C	3.992047	9.802143	4.252770
C	5.676323	9.387841	−0.223424
H	4.932981	10.572380	1.945067
C	2.219906	10.605577	−1.162244
H	1.717952	12.110825	0.319070
C	2.647908	11.498335	−2.177274
C	2.259034	9.210502	−1.420325
C	1.826828	8.314269	−0.406607
H	1.861156	7.251284	−0.616590
C	3.108064	11.021876	−3.382838
H	2.619298	12.567957	−1.980447
H	3.438479	11.716835	−4.149561
C	3.157980	9.631793	−3.634970
C	2.735398	8.748693	−2.672020
H	3.521628	9.263314	−4.589022
H	2.763643	7.677953	−2.859274
C	−0.392349	9.364683	5.555540
H	0.071230	11.295228	4.689855

C	−0.843563	9.852208	6.806088
C	−0.397401	7.966273	5.318292
C	0.079066	7.472966	4.075189
H	0.107676	6.398064	3.937384
C	−1.283020	8.987854	7.780132
H	−0.832098	10.924871	6.983223
H	−1.627059	9.373381	8.735018
C	−1.296342	7.594766	7.541557
C	−0.861865	7.098150	6.336147
H	−1.652261	6.918957	8.313085
H	−0.865700	6.027129	6.146797
C	3.463871	9.222402	5.435858
H	4.264201	10.855403	4.252586
C	3.141408	7.838931	5.433425
C	3.314590	7.094849	4.233116
C	2.600905	7.256012	6.603693
H	3.024826	6.047292	4.220987
C	5.939307	8.644071	−1.400244
H	6.025971	10.415646	−0.156690
C	5.429633	7.322872	−1.498673
C	4.694678	6.787458	−0.404525
C	5.674492	6.584014	−2.682019
H	4.278420	5.788911	−0.490453
C	2.378220	8.011270	7.729899
H	2.336309	6.201166	6.587088
H	1.935497	7.558279	8.611068
C	2.696557	9.387323	7.731530
C	3.231347	9.977440	6.611397
H	2.505764	9.980584	8.620610
H	3.472694	11.037521	6.607459
C	6.404992	7.122037	−3.715191
H	5.287050	5.572400	−2.768824
H	6.600267	6.531295	−4.605332
C	6.906563	8.439579	−3.615132
C	6.674396	9.183095	−2.483626
H	7.476021	8.862277	−4.437221

H	7.049884	10.200036	−2.403272
C	0.310676	5.549396	1.642569
C	1.346283	6.475153	1.704400
H	−0.722570	5.879665	1.675825
C	2.707809	6.041718	1.672236
C	3.011267	4.685549	1.586349
H	4.042557	4.350158	1.604506
C	−2.304499	1.930277	1.570278
C	−3.767678	1.963658	1.564064
N	−7.014457	3.732438	1.837075
C	−4.196701	0.630413	1.589538
N	−7.855320	1.054370	1.858820
C	−2.994672	−0.201784	1.582425
N	−1.531417	3.011094	1.579821
N	−1.907832	0.623187	1.577230
C	−8.313663	0.528050	3.086447
C	−8.747724	1.433585	0.832706
C	−10.155404	1.384734	1.084693
C	−9.727680	0.505671	3.323311
N	−10.580202	0.966108	2.331285
C	−11.044033	1.761565	0.107395
C	−10.220006	0.067693	4.525266
H	−11.561769	0.756285	2.441618
C	−7.504964	4.480163	0.741638
C	−7.693725	3.740728	3.076344
C	−9.068869	4.136632	3.101869
C	−8.853077	4.960129	0.815837
N	−9.609114	4.631666	1.931171
C	−9.802143	3.992047	4.252770
C	−9.387841	5.676323	−0.223424
H	−10.572380	4.932981	1.945067
C	−10.605577	2.219906	−1.162244
H	−12.110825	1.717952	0.319070
C	−11.498335	2.647908	−2.177274
C	−9.210502	2.259034	−1.420325
C	−8.314269	1.826828	−0.406607

H	−7.251284	1.861156	−0.616590
C	−11.021876	3.108064	−3.382838
H	−12.567957	2.619298	−1.980447
H	−11.716835	3.438479	−4.149561
C	−9.631793	3.157980	−3.634970
C	−8.748693	2.735398	−2.672020
H	−9.263314	3.521628	−4.589022
H	−7.677953	2.763643	−2.859274
C	−9.364683	−0.392349	5.555540
H	−11.295228	0.071230	4.689855
C	−9.852208	−0.843563	6.806088
C	−7.966273	−0.397401	5.318292
C	−7.472966	0.079066	4.075189
H	−6.398064	0.107676	3.937384
C	−8.987854	−1.283020	7.780132
H	−10.924871	−0.832098	6.983223
H	−9.373381	−1.627059	8.735018
C	−7.594766	−1.296342	7.541557
C	−7.098150	−0.861865	6.336147
H	−6.918957	−1.652261	8.313085
H	−6.027129	−0.865700	6.146797
C	−9.222402	3.463871	5.435858
H	−10.855403	4.264201	4.252586
C	−7.838931	3.141408	5.433425
C	−7.094849	3.314590	4.233116
C	−7.256012	2.600905	6.603693
H	−6.047292	3.024826	4.220987
C	−8.644071	5.939307	−1.400244
H	−10.415646	6.025971	−0.156690
C	−7.322872	5.429633	−1.498673
C	−6.787458	4.694678	−0.404525
C	−6.584014	5.674492	−2.682019
H	−5.788911	4.278420	−0.490453
C	−8.011270	2.378220	7.729899
H	−6.201166	2.336309	6.587088
H	−7.558279	1.935497	8.611068

C	−9.387323	2.696557	7.731530
C	−9.977440	3.231347	6.611397
H	−9.980584	2.505764	8.620610
H	−11.037521	3.472694	6.607459
C	−7.122037	6.404992	−3.715191
H	−5.572400	5.287050	−2.768824
H	−6.531295	6.600267	−4.605332
C	−8.439579	6.906563	−3.615132
C	−9.183095	6.674396	−2.483626
H	−8.862277	7.476021	−4.437221
H	−10.200036	7.049884	−2.403272
C	−5.549396	0.310676	1.642569
C	−6.475153	1.346283	1.704400
H	−5.879665	−0.722570	1.675825
C	−6.041718	2.707809	1.672236
C	−4.685549	3.011267	1.586349
H	−4.350158	4.042557	1.604506
C	−1.930277	−2.304499	1.570278
C	−1.963658	−3.767678	1.564064
N	−3.732438	−7.014457	1.837075
C	−0.630413	−4.196701	1.589538
N	−1.054370	−7.855320	1.858820
C	0.201784	−2.994672	1.582425
N	−3.011094	−1.531417	1.579821
N	−0.623187	−1.907832	1.577230
C	−0.528050	−8.313663	3.086447
C	−1.433585	−8.747724	0.832706
C	−1.384734	−10.155404	1.084693
C	−0.505671	−9.727680	3.323311
N	−0.966108	−10.580202	2.331285
C	−1.761565	−11.044033	0.107395
C	−0.067693	−10.220006	4.525266
H	−0.756285	−11.561769	2.441618
C	−4.480163	−7.504964	0.741638
C	−3.740728	−7.693725	3.076344
C	−4.136632	−9.068869	3.101869

C	−4.960129	−8.853077	0.815837
N	−4.631666	−9.609114	1.931171
C	−3.992047	−9.802143	4.252770
C	−5.676323	−9.387841	−0.223424
H	−4.932981	−10.572380	1.945067
C	−2.219906	−10.605577	−1.162244
H	−1.717952	−12.110825	0.319070
C	−2.647908	−11.498335	−2.177274
C	−2.259034	−9.210502	−1.420325
C	−1.826828	−8.314269	−0.406607
H	−1.861156	−7.251284	−0.616590
C	−3.108064	−11.021876	−3.382838
H	−2.619298	−12.567957	−1.980447
H	−3.438479	−11.716835	−4.149561
C	−3.157980	−9.631793	−3.634970
C	−2.735398	−8.748693	−2.672020
H	−3.521628	−9.263314	−4.589022
H	−2.763643	−7.677953	−2.859274
C	0.392349	−9.364683	5.555540
H	−0.071230	−11.295228	4.689855
C	0.843563	−9.852208	6.806088
C	0.397401	−7.966273	5.318292
C	−0.079066	−7.472966	4.075189
H	−0.107676	−6.398064	3.937384
C	1.283020	−8.987854	7.780132
H	0.832098	−10.924871	6.983223
H	1.627059	−9.373381	8.735018
C	1.296342	−7.594766	7.541557
C	0.861865	−7.098150	6.336147
H	1.652261	−6.918957	8.313085
H	0.865700	−6.027129	6.146797
C	−3.463871	−9.222402	5.435858
H	−4.264201	−10.855403	4.252586
C	−3.141408	−7.838931	5.433425
C	−3.314590	−7.094849	4.233116
C	−2.600905	−7.256012	6.603693

H	−3.024826	−6.047292	4.220987
C	−5.939307	−8.644071	−1.400244
H	−6.025971	−10.415646	−0.156690
C	−5.429633	−7.322872	−1.498673
C	−4.694678	−6.787458	−0.404525
C	−5.674492	−6.584014	−2.682019
H	−4.278420	−5.788911	−0.490453
C	−2.378220	−8.011270	7.729899
H	−2.336309	−6.201166	6.587088
H	−1.935497	−7.558279	8.611068
C	−2.696557	−9.387323	7.731530
C	−3.231347	−9.977440	6.611397
H	−2.505764	−9.980584	8.620610
H	−3.472694	−11.037521	6.607459
C	−6.404992	−7.122037	−3.715191
H	−5.287050	−5.572400	−2.768824
H	−6.600267	−6.531295	−4.605332
C	−6.906563	−8.439579	−3.615132
C	−6.674396	−9.183095	−2.483626
H	−7.476021	−8.862277	−4.437221
H	−7.049884	−10.200036	−2.403272
C	−0.310676	−5.549396	1.642569
C	−1.346283	−6.475153	1.704400
H	0.722570	−5.879665	1.675825
C	−2.707809	−6.041718	1.672236
C	−3.011267	−4.685549	1.586349
H	−4.042557	−4.350158	1.604506
C	2.304499	−1.930277	1.570278
C	3.767678	−1.963658	1.564064
N	7.014457	−3.732438	1.837075
C	4.196701	−0.630413	1.589538
N	7.855320	−1.054370	1.858820
C	2.994672	0.201784	1.582425
N	1.531417	−3.011094	1.579821
N	1.907832	−0.623187	1.577230
C	8.313663	−0.528050	3.086447

C	8.747724	−1.433585	0.832706
C	10.155404	−1.384734	1.084693
C	9.727680	−0.505671	3.323311
N	10.580202	−0.966108	2.331285
C	11.044033	−1.761565	0.107395
C	10.220006	−0.067693	4.525266
H	11.561769	−0.756285	2.441618
C	7.504964	−4.480163	0.741638
C	7.693725	−3.740728	3.076344
C	9.068869	−4.136632	3.101869
C	8.853077	−4.960129	0.815837
N	9.609114	−4.631666	1.931171
C	9.802143	−3.992047	4.252770
C	9.387841	−5.676323	−0.223424
H	10.572380	−4.932981	1.945067
C	10.605577	−2.219906	−1.162244
H	12.110825	−1.717952	0.319070
C	11.498335	−2.647908	−2.177274
C	9.210502	−2.259034	−1.420325
C	8.314269	−1.826828	−0.406607
H	7.251284	−1.861156	−0.616590
C	11.021876	−3.108064	−3.382838
H	12.567957	−2.619298	−1.980447
H	11.716835	−3.438479	−4.149561
C	9.631793	−3.157980	−3.634970
C	8.748693	−2.735398	−2.672020
H	9.263314	−3.521628	−4.589022
H	7.677953	−2.763643	−2.859274
C	9.364683	0.392349	5.555540
H	11.295228	−0.071230	4.689855
C	9.852208	0.843563	6.806088
C	7.966273	0.397401	5.318292
C	7.472966	−0.079066	4.075189
H	6.398064	−0.107676	3.937384
C	8.987854	1.283020	7.780132
H	10.924871	0.832098	6.983223

H	9.373381	1.627059	8.735018
C	7.594766	1.296342	7.541557
C	7.098150	0.861865	6.336147
H	6.918957	1.652261	8.313085
H	6.027129	0.865700	6.146797
C	9.222402	-3.463871	5.435858
H	10.855403	-4.264201	4.252586
C	7.838931	-3.141408	5.433425
C	7.094849	-3.314590	4.233116
C	7.256012	-2.600905	6.603693
H	6.047292	-3.024826	4.220987
C	8.644071	-5.939307	-1.400244
H	10.415646	-6.025971	-0.156690
C	7.322872	-5.429633	-1.498673
C	6.787458	-4.694678	-0.404525
C	6.584014	-5.674492	-2.682019
H	5.788911	-4.278420	-0.490453
C	8.011270	-2.378220	7.729899
H	6.201166	-2.336309	6.587088
H	7.558279	-1.935497	8.611068
C	9.387323	-2.696557	7.731530
C	9.977440	-3.231347	6.611397
H	9.980584	-2.505764	8.620610
H	11.037521	-3.472694	6.607459
C	7.122037	-6.404992	-3.715191
H	5.572400	-5.287050	-2.768824
H	6.531295	-6.600267	-4.605332
C	8.439579	-6.906563	-3.615132
C	9.183095	-6.674396	-2.483626
H	8.862277	-7.476021	-4.437221
H	10.200036	-7.049884	-2.403272
C	5.549396	-0.310676	1.642569
C	6.475153	-1.346283	1.704400
H	5.879665	0.722570	1.675825
C	6.041718	-2.707809	1.672236
C	4.685549	-3.011267	1.586349

H	4.350158	−4.042557	1.604506
Zn	0.000000	0.000000	1.674967
C	2.994672	−0.201784	−1.582425
C	4.196701	0.630413	−1.589538
N	7.855320	1.054370	−1.858820
C	3.767678	1.963658	−1.564064
N	7.014457	3.732438	−1.837075
C	2.304499	1.930277	−1.570278
N	3.011094	−1.531417	−1.579821
N	1.907832	0.623187	−1.577230
C	7.504964	4.480163	−0.741638
C	7.693725	3.740728	−3.076344
C	9.068869	4.136632	−3.101869
C	8.853077	4.960129	−0.815837
N	9.609114	4.631666	−1.931171
C	9.802143	3.992047	−4.252770
C	9.387841	5.676323	0.223424
H	10.572380	4.932981	−1.945067
C	8.313663	0.528050	−3.086447
C	8.747724	1.433585	−0.832706
C	10.155404	1.384734	−1.084693
C	9.727680	0.505671	−3.323311
N	10.580202	0.966108	−2.331285
C	11.044033	1.761565	−0.107395
C	10.220006	0.067693	−4.525266
H	11.561769	0.756285	−2.441618
C	9.222402	3.463871	−5.435858
H	10.855403	4.264201	−4.252586
C	9.977440	3.231347	−6.611397
C	7.838931	3.141408	−5.433425
C	7.094849	3.314590	−4.233116
H	6.047292	3.024826	−4.220987
C	9.387323	2.696557	−7.731530
H	11.037521	3.472694	−6.607459
H	9.980584	2.505764	−8.620610
C	8.011270	2.378220	−7.729899

C	7.256012	2.600905	−6.603693
H	7.558279	1.935497	−8.611068
H	6.201166	2.336309	−6.587088
C	8.644071	5.939307	1.400244
H	10.415646	6.025971	0.156690
C	9.183095	6.674396	2.483626
C	7.322872	5.429633	1.498673
C	6.787458	4.694678	0.404525
H	5.788911	4.278420	0.490453
C	8.439579	6.906563	3.615132
H	10.200036	7.049884	2.403272
H	8.862277	7.476021	4.437221
C	7.122037	6.404992	3.715191
C	6.584014	5.674492	2.682019
H	6.531295	6.600267	4.605332
H	5.572400	5.287050	2.768824
C	10.605577	2.219906	1.162244
H	12.110825	1.717952	−0.319070
C	9.210502	2.259034	1.420325
C	8.314269	1.826828	0.406607
C	8.748693	2.735398	2.672020
H	7.251284	1.861156	0.616590
C	9.364683	−0.392349	−5.555540
H	11.295228	0.071230	−4.689855
C	7.966273	−0.397401	−5.318292
C	7.472966	0.079066	−4.075189
C	7.098150	−0.861865	−6.336147
H	6.398064	0.107676	−3.937384
C	9.631793	3.157980	3.634970
H	7.677953	2.763643	2.859274
H	9.263314	3.521628	4.589022
C	11.021876	3.108064	3.382838
C	11.498335	2.647908	2.177274
H	11.716835	3.438479	4.149561
H	12.567957	2.619298	1.980447
C	7.594766	−1.296342	−7.541557

H	6.027129	−0.865700	−6.146797
H	6.918957	−1.652261	−8.313085
C	8.987854	−1.283020	−7.780132
C	9.852208	−0.843563	−6.806088
H	9.373381	−1.627059	−8.735018
H	10.924871	−0.832098	−6.983223
C	4.685549	3.011267	−1.586349
C	6.041718	2.707809	−1.672236
H	4.350158	4.042557	−1.604506
C	6.475153	1.346283	−1.704400
C	5.549396	0.310676	−1.642569
H	5.879665	−0.722570	−1.675825
C	0.201784	2.994672	−1.582425
C	−0.630413	4.196701	−1.589538
N	−1.054370	7.855320	−1.858820
C	−1.963658	3.767678	−1.564064
N	−3.732438	7.014457	−1.837075
C	−1.930277	2.304499	−1.570278
N	1.531417	3.011094	−1.579821
N	−0.623187	1.907832	−1.577230
C	−4.480163	7.504964	−0.741638
C	−3.740728	7.693725	−3.076344
C	−4.136632	9.068869	−3.101869
C	−4.960129	8.853077	−0.815837
N	−4.631666	9.609114	−1.931171
C	−3.992047	9.802143	−4.252770
C	−5.676323	9.387841	0.223424
H	−4.932981	10.572380	−1.945067
C	−0.528050	8.313663	−3.086447
C	−1.433585	8.747724	−0.832706
C	−1.384734	10.155404	−1.084693
C	−0.505671	9.727680	−3.323311
N	−0.966108	10.580202	−2.331285
C	−1.761565	11.044033	−0.107395
C	−0.067693	10.220006	−4.525266
H	−0.756285	11.561769	−2.441618

C	−3.463871	9.222402	−5.435858
H	−4.264201	10.855403	−4.252586
C	−3.231347	9.977440	−6.611397
C	−3.141408	7.838931	−5.433425
C	−3.314590	7.094849	−4.233116
H	−3.024826	6.047292	−4.220987
C	−2.696557	9.387323	−7.731530
H	−3.472694	11.037521	−6.607459
H	−2.505764	9.980584	−8.620610
C	−2.378220	8.011270	−7.729899
C	−2.600905	7.256012	−6.603693
H	−1.935497	7.558279	−8.611068
H	−2.336309	6.201166	−6.587088
C	−5.939307	8.644071	1.400244
H	−6.025971	10.415646	0.156690
C	−6.674396	9.183095	2.483626
C	−5.429633	7.322872	1.498673
C	−4.694678	6.787458	0.404525
H	−4.278420	5.788911	0.490453
C	−6.906563	8.439579	3.615132
H	−7.049884	10.200036	2.403272
H	−7.476021	8.862277	4.437221
C	−6.404992	7.122037	3.715191
C	−5.674492	6.584014	2.682019
H	−6.600267	6.531295	4.605332
H	−5.287050	5.572400	2.768824
C	−2.219906	10.605577	1.162244
H	−1.717952	12.110825	−0.319070
C	−2.259034	9.210502	1.420325
C	−1.826828	8.314269	0.406607
C	−2.735398	8.748693	2.672020
H	−1.861156	7.251284	0.616590
C	0.392349	9.364683	−5.555540
H	−0.071230	11.295228	−4.689855
C	0.397401	7.966273	−5.318292
C	−0.079066	7.472966	−4.075189

C	0.861865	7.098150	−6.336147
H	−0.107676	6.398064	−3.937384
C	−3.157980	9.631793	3.634970
H	−2.763643	7.677953	2.859274
H	−3.521628	9.263314	4.589022
C	−3.108064	11.021876	3.382838
C	−2.647908	11.498335	2.177274
H	−3.438479	11.716835	4.149561
H	−2.619298	12.567957	1.980447
C	1.296342	7.594766	−7.541557
H	0.865700	6.027129	−6.146797
H	1.652261	6.918957	−8.313085
C	1.283020	8.987854	−7.780132
C	0.843563	9.852208	−6.806088
H	1.627059	9.373381	−8.735018
H	0.832098	10.924871	−6.983223
C	−3.011267	4.685549	−1.586349
C	−2.707809	6.041718	−1.672236
H	−4.042557	4.350158	−1.604506
C	−1.346283	6.475153	−1.704400
C	−0.310676	5.549396	−1.642569
H	0.722570	5.879665	−1.675825
C	−2.994672	0.201784	−1.582425
C	−4.196701	−0.630413	−1.589538
N	−7.855320	−1.054370	−1.858820
C	−3.767678	−1.963658	−1.564064
N	−7.014457	−3.732438	−1.837075
C	−2.304499	−1.930277	−1.570278
N	−3.011094	1.531417	−1.579821
N	−1.907832	−0.623187	−1.577230
C	−7.504964	−4.480163	−0.741638
C	−7.693725	−3.740728	−3.076344
C	−9.068869	−4.136632	−3.101869
C	−8.853077	−4.960129	−0.815837
N	−9.609114	−4.631666	−1.931171
C	−9.802143	−3.992047	−4.252770

C	−9.387841	−5.676323	0.223424
H	−10.572380	−4.932981	−1.945067
C	−8.313663	−0.528050	−3.086447
C	−8.747724	−1.433585	−0.832706
C	−10.155404	−1.384734	−1.084693
C	−9.727680	−0.505671	−3.323311
N	−10.580202	−0.966108	−2.331285
C	−11.044033	−1.761565	−0.107395
C	−10.220006	−0.067693	−4.525266
H	−11.561769	−0.756285	−2.441618
C	−9.222402	−3.463871	−5.435858
H	−10.855403	−4.264201	−4.252586
C	−9.977440	−3.231347	−6.611397
C	−7.838931	−3.141408	−5.433425
C	−7.094849	−3.314590	−4.233116
H	−6.047292	−3.024826	−4.220987
C	−9.387323	−2.696557	−7.731530
H	−11.037521	−3.472694	−6.607459
H	−9.980584	−2.505764	−8.620610
C	−8.011270	−2.378220	−7.729899
C	−7.256012	−2.600905	−6.603693
H	−7.558279	−1.935497	−8.611068
H	−6.201166	−2.336309	−6.587088
C	−8.644071	−5.939307	1.400244
H	−10.415646	−6.025971	0.156690
C	−9.183095	−6.674396	2.483626
C	−7.322872	−5.429633	1.498673
C	−6.787458	−4.694678	0.404525
H	−5.788911	−4.278420	0.490453
C	−8.439579	−6.906563	3.615132
H	−10.200036	−7.049884	2.403272
H	−8.862277	−7.476021	4.437221
C	−7.122037	−6.404992	3.715191
C	−6.584014	−5.674492	2.682019
H	−6.531295	−6.600267	4.605332
H	−5.572400	−5.287050	2.768824

C	−10.605577	−2.219906	1.162244
H	−12.110825	−1.717952	−0.319070
C	−9.210502	−2.259034	1.420325
C	−8.314269	−1.826828	0.406607
C	−8.748693	−2.735398	2.672020
H	−7.251284	−1.861156	0.616590
C	−9.364683	0.392349	−5.555540
H	−11.295228	−0.071230	−4.689855
C	−7.966273	0.397401	−5.318292
C	−7.472966	−0.079066	−4.075189
C	−7.098150	0.861865	−6.336147
H	−6.398064	−0.107676	−3.937384
C	−9.631793	−3.157980	3.634970
H	−7.677953	−2.763643	2.859274
H	−9.263314	−3.521628	4.589022
C	−11.021876	−3.108064	3.382838
C	−11.498335	−2.647908	2.177274
H	−11.716835	−3.438479	4.149561
H	−12.567957	−2.619298	1.980447
C	−7.594766	1.296342	−7.541557
H	−6.027129	0.865700	−6.146797
H	−6.918957	1.652261	−8.313085
C	−8.987854	1.283020	−7.780132
C	−9.852208	0.843563	−6.806088
H	−9.373381	1.627059	−8.735018
H	−10.924871	0.832098	−6.983223
C	−4.685549	−3.011267	−1.586349
C	−6.041718	−2.707809	−1.672236
H	−4.350158	−4.042557	−1.604506
C	−6.475153	−1.346283	−1.704400
C	−5.549396	−0.310676	−1.642569
H	−5.879665	0.722570	−1.675825
C	−0.201784	−2.994672	−1.582425
C	0.630413	−4.196701	−1.589538
N	1.054370	−7.855320	−1.858820
C	1.963658	−3.767678	−1.564064

N	3.732438	−7.014457	−1.837075
C	1.930277	−2.304499	−1.570278
N	−1.531417	−3.011094	−1.579821
N	0.623187	−1.907832	−1.577230
C	4.480163	−7.504964	−0.741638
C	3.740728	−7.693725	−3.076344
C	4.136632	−9.068869	−3.101869
C	4.960129	−8.853077	−0.815837
N	4.631666	−9.609114	−1.931171
C	3.992047	−9.802143	−4.252770
C	5.676323	−9.387841	0.223424
H	4.932981	−10.572380	−1.945067
C	0.528050	−8.313663	−3.086447
C	1.433585	−8.747724	−0.832706
C	1.384734	−10.155404	−1.084693
C	0.505671	−9.727680	−3.323311
N	0.966108	−10.580202	−2.331285
C	1.761565	−11.044033	−0.107395
C	0.067693	−10.220006	−4.525266
H	0.756285	−11.561769	−2.441618
C	3.463871	−9.222402	−5.435858
H	4.264201	−10.855403	−4.252586
C	3.231347	−9.977440	−6.611397
C	3.141408	−7.838931	−5.433425
C	3.314590	−7.094849	−4.233116
H	3.024826	−6.047292	−4.220987
C	2.696557	−9.387323	−7.731530
H	3.472694	−11.037521	−6.607459
H	2.505764	−9.980584	−8.620610
C	2.378220	−8.011270	−7.729899
C	2.600905	−7.256012	−6.603693
H	1.935497	−7.558279	−8.611068
H	2.336309	−6.201166	−6.587088
C	5.939307	−8.644071	1.400244
H	6.025971	−10.415646	0.156690
C	6.674396	−9.183095	2.483626

C	5.429633	−7.322872	1.498673
C	4.694678	−6.787458	0.404525
H	4.278420	−5.788911	0.490453
C	6.906563	−8.439579	3.615132
H	7.049884	−10.200036	2.403272
H	7.476021	−8.862277	4.437221
C	6.404992	−7.122037	3.715191
C	5.674492	−6.584014	2.682019
H	6.600267	−6.531295	4.605332
H	5.287050	−5.572400	2.768824
C	2.219906	−10.605577	1.162244
H	1.717952	−12.110825	−0.319070
C	2.259034	−9.210502	1.420325
C	1.826828	−8.314269	0.406607
C	2.735398	−8.748693	2.672020
H	1.861156	−7.251284	0.616590
C	−0.392349	−9.364683	−5.555540
H	0.071230	−11.295228	−4.689855
C	−0.397401	−7.966273	−5.318292
C	0.079066	−7.472966	−4.075189
C	−0.861865	−7.098150	−6.336147
H	0.107676	−6.398064	−3.937384
C	3.157980	−9.631793	3.634970
H	2.763643	−7.677953	2.859274
H	3.521628	−9.263314	4.589022
C	3.108064	−11.021876	3.382838
C	2.647908	−11.498335	2.177274
H	3.438479	−11.716835	4.149561
H	2.619298	−12.567957	1.980447
C	−1.296342	−7.594766	−7.541557
H	−0.865700	−6.027129	−6.146797
H	−1.652261	−6.918957	−8.313085
C	−1.283020	−8.987854	−7.780132
C	−0.843563	−9.852208	−6.806088
H	−1.627059	−9.373381	−8.735018
H	−0.832098	−10.924871	−6.983223

C	3.011267	−4.685549	−1.586349
C	2.707809	−6.041718	−1.672236
H	4.042557	−4.350158	−1.604506
C	1.346283	−6.475153	−1.704400
C	0.310676	−5.549396	−1.642569
H	−0.722570	−5.879665	−1.675825
Zn	0.000000	0.000000	−1.674967

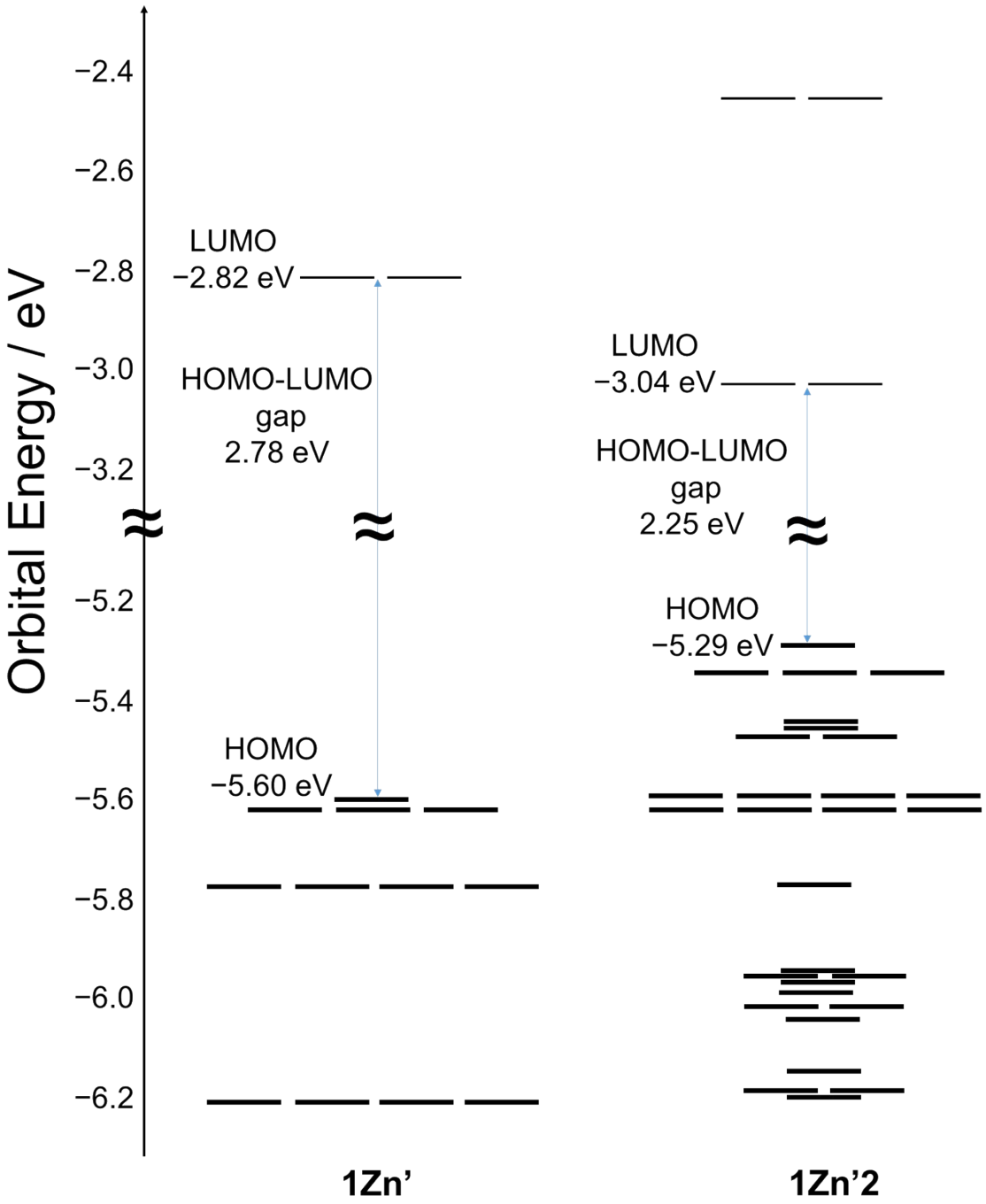

Figure S38. MO diagrams of **1Zn'** and **1Zn'2** calculated at M06-2X/6-31G*, LANL2DZ.