Electronic Supplementary Information (ESI) for:

A square-shaped complex with an electron-acceptor ligand: unique cubic crystal symmetry and similarity to the inorganic mineral katoite

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1. Synthesis.

Monitoring the reaction of the square macrocyclic complex $[Pt(en)(dpndi)]_4(NO_3)_8$

After a 1-week reaction, more than three peaks probably due to the oligomers were observed, and formation of the macrocyclic complex was not clearly confirmed (Fig. S2). As the reaction proceeds further and after a 2-week reaction, the number of peaks turned to three, the same number as free dpndi, and a peak shift was observed compared with the free dpndi. This clearly implied the formation of the metal–ligand bonds. Moreover, the H^a peak split into two, which were assigned to the square and triangular macrocyclic complexes. For H^b and H^c, the peaks of square and triangular macrocyclic complexes greatly overlapped. In the syntheses of the Pt-based square macrocyclic complexes, it is often the case that an enthalpically favourable square macrocyclic complex and an entropically favourable triangular macrocyclic complex compete with each other (Fig. S4).[1] As time goes by, the reaction reaches the equilibrium, and the square macrocyclic complex becomes the major product. The peaks of the square and triangular macrocyclic complex were assigned in accordance with the previous report,[1] and the integral ratios between the square and triangular macrocyclic complexes calculated from H^a were 10:7 and 5:2 for the 2-week and 3-week reactions, respectively. In the 4-week reaction, the integral ratio does not change anymore, hence it is concluded that the reaction reaches equilibrium in 3 weeks.

^{1}H NMR for 2-week reaction: δ= 9.22 (*d*, □-H^a), 9.19 (*d*, △-H^a), 8.76 (*d*, (□+△)-H^c),
7.92 (*d*, (□+△)-H^b), with □:△ = 10:7
6.46 (br, NH_2 of en), 2.69 (br, CH_2 of en)

^{1}H NMR for 3-week reaction: δ= 9.22 (*d*, □-H^a), 9.17 (*d*, △-H^a), 8.76 (*d*, (□+△)-H^c),
7.94 (*d*, (□+△)-H^b), with □:△ = 5:2
6.45 (br, NH_2 of en), 2.69 (br, CH_2 of en)

^{1}H NMR for single crystals of **1**: δ= 9.21 (*d*, □-H^a), 8.76 (*s*, □-H^c), 7.94 (*d*, □-H^b),
6.46 (br, NH_2 of en), 2.69 (br, CH_2 of en)

Elemental analysis:
Anal. calcd for $[Pt(en)(dpndi)]_4(SO_4)_4 \cdot 20H_2O$: C, 35.47%; H, 3.67%; N, 9.22%.
Found: C, 35.79%; H, 3.50%; N, 9.45%

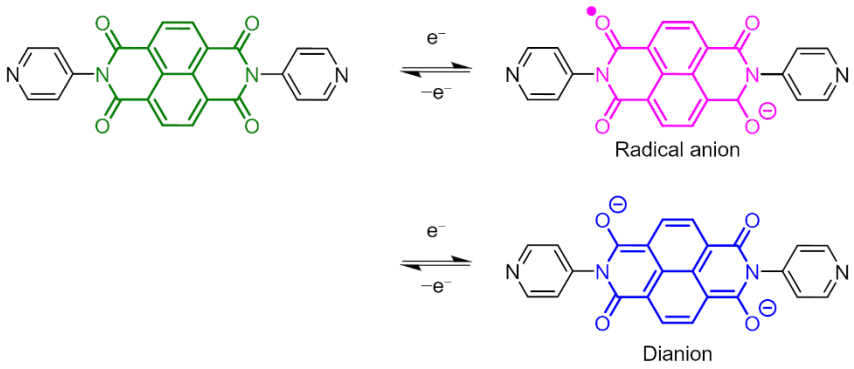

Fig. S1 Structure of dpndi (left), and radical anion and dianion states (right) by accepting two electrons.

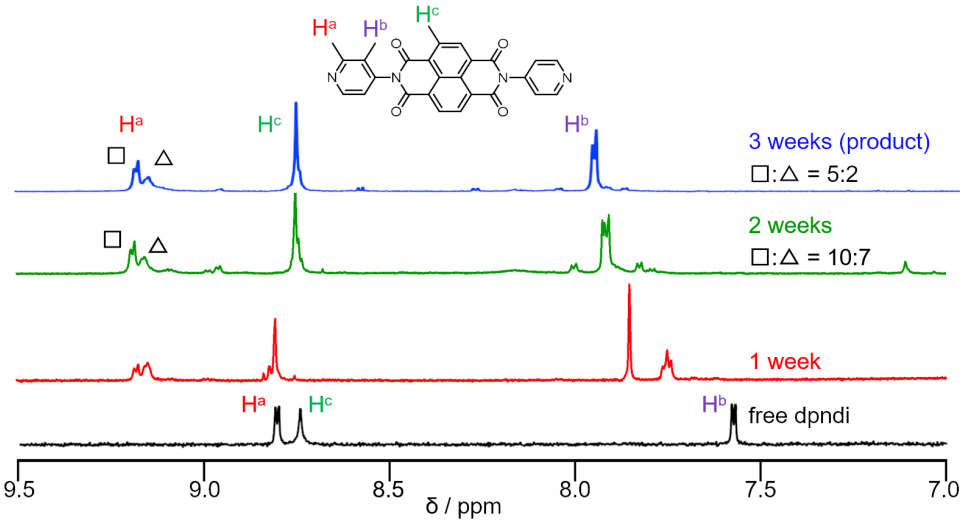

Fig. S2 ^{1}H NMR spectra in the aromatic region for free dpndi (black) and after 1-, (red), 2- (green), and 3-week (blue) reactions in DMSO-d_6.

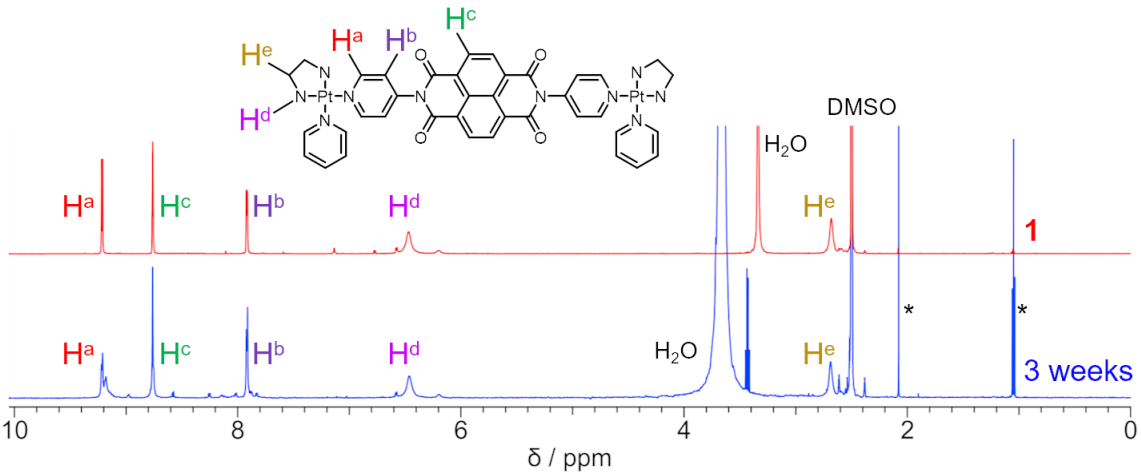

Fig. S3 Full range ^{1}H NMR spectra after a 3-week reaction (blue) and anion exchanged to SO_4^{2-} (red) in DMSO-d_6. Asterisks denote the impurity peaks of the deuterated solvent.

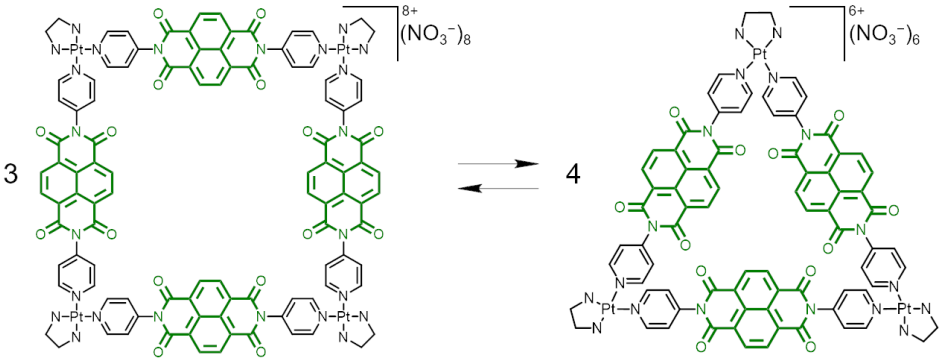

Fig. S4 Equilibrium between the square and triangular macrocyclic complexes.

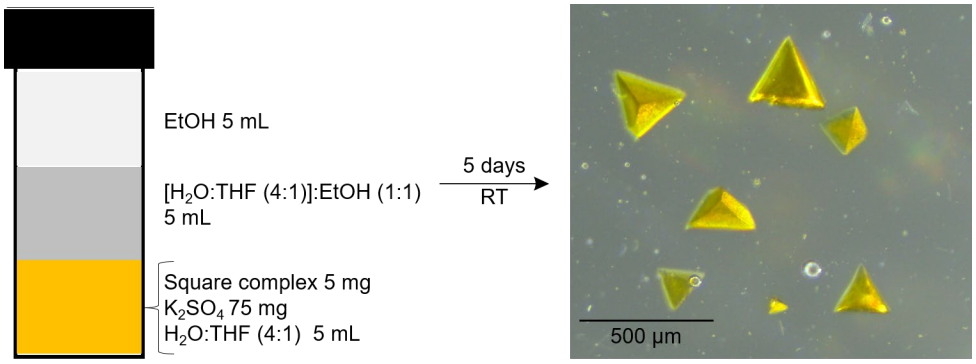

Fig. S5 Synthetic scheme (left) and photograph of single crystals of **1** dispersed in Paraton-N oil (right).

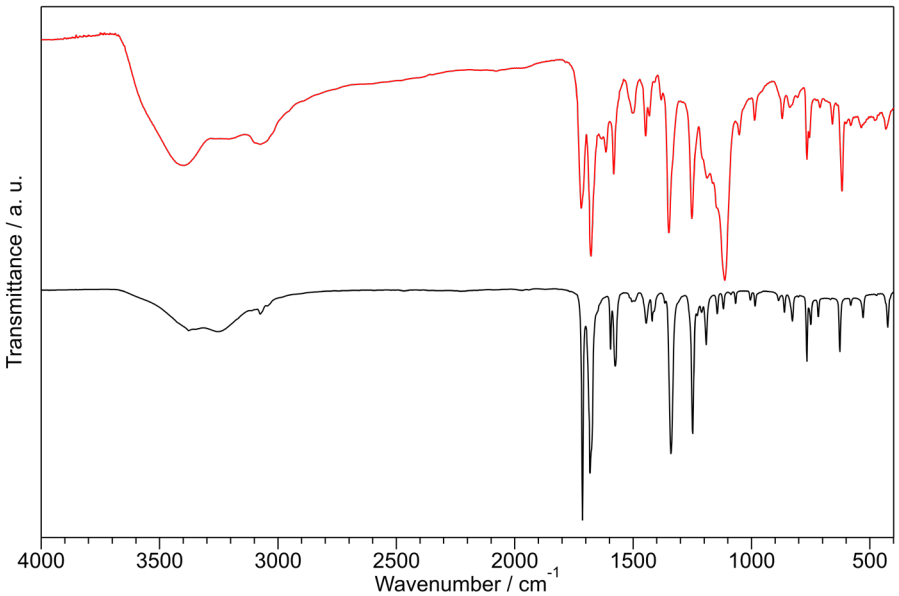

Fig. S6 IR spectra of dpndi (black) and **1** (red) diluted in KBr. Peak assignments of **1** are as follows: ν(O–H stretching mode) 3700–3350 cm^{-1}, ν(N–H stretching mode) 3300–3100 cm^{-1}, ν(O–H stretching mode) 3100–2850 cm^{-1}, ν(C=O stretching) 1720 and 1678 cm^{-1}, ν(imide stretching) 1581 cm^{-1}, ν(C=C stretching) 1340 cm^{-1}, ν(C–N stretching) 1251 cm^{-1}, ν(S–O stretching) 1112 cm^{-1}, δ(S–O bending) 617 cm^{-1}.

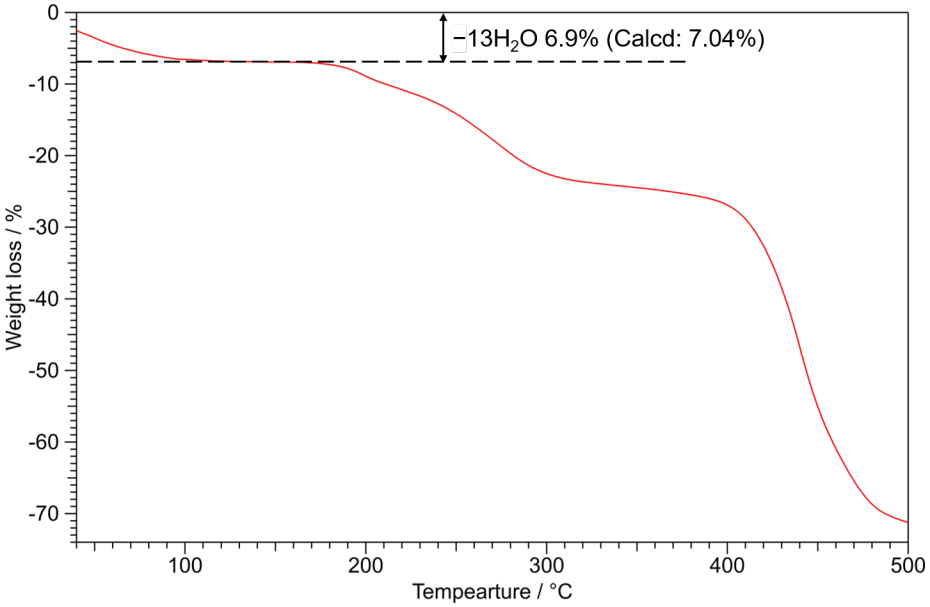

Fig. S7 TGA of **1**. The first weight loss (approximately 6.9%) was observed at approximately 100 ˚C due to the desorption of H_2O (Calcd 7.04% for −13 H_2O). The inconsistency of the number of the water with elemental analysis (20 H_2O), and weight loss from the start probably originated from the loss of the crystallization water after loading the sample to the measurement setup.

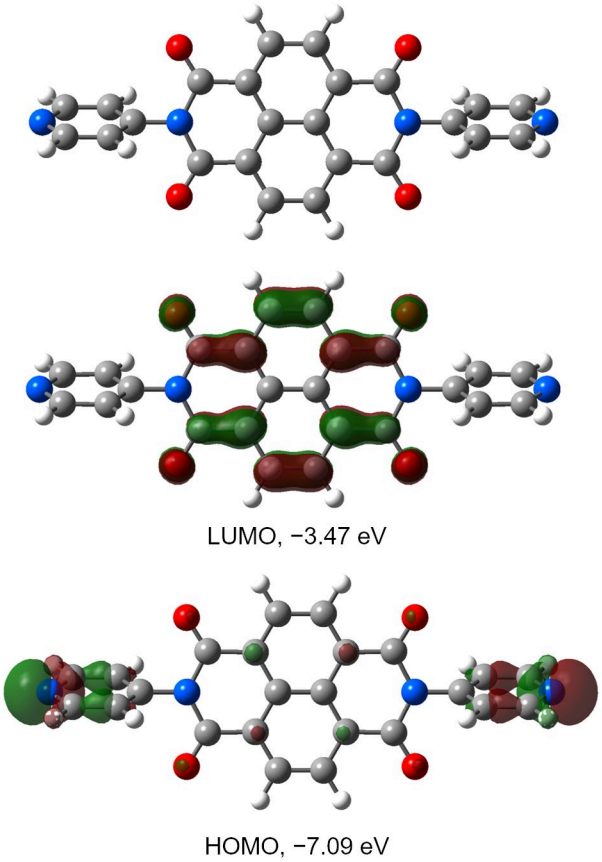

Fig. S8 Optimized structure, HOMO and LUMO of dpndi. LUMO is localized to the electron accepting moiety. The values below the orbitals denote the energy levels.

2. Structural Analysis.

The solvent-accessible voids in the unit cell (63782 Å^3) among the square units and SO_4^{2-} anions were calculated to be 36522 Å^3 (57.3%) according to PLATON software.[2] Because of the severe disorder of the solvent molecules, no electron density corresponding to the solvent molecules could be found (less than 3.0 e/Å^3) before the SQUEEZE routine and the refinement. The following is the details of the SQUEEZE result.

TITL shelxl I −4 3 d R = 0.07
CELL 39.9546 39.9546 39.9546 90.00 90.00 90.00
SPGR I−43d
Solvent Accessible Volume = 36522
Electrons Found in S.A.V. = 16227
Note: Atoms in Void as Cxxx and Qxxx all others
Q101 0.974 0.698 0.124 ! 6.04 e A^{-3}
C102 0.405 0.197 0.123 ! 5.75 e A^{-3}
C103 0.605 0.556 0.370 ! 4.85 e A^{-3}
Q104 0.673 0.455 0.375 ! 4.69 e A^{-3}
C105 0.063 0.069 0.399 ! 4.57 e A^{-3}
C106 0.818 0.017 0.047 ! 4.35 e A^{-3}
C107 0.375 0.375 0.375 ! 4.21 e A^{-3}
C108 0.875 0.875 0.875 ! 4.21 e A^{-3}
C109 0.157 0.541 0.210 ! 4.16 e A^{-3}
C110 0.055 0.703 0.249 ! 3.89 e A^{-3}
C111 0.227 0.694 0.126 ! 3.59 eA^{-3}
C112 0.092 0.048 0.050 ! 3.57 e A^{-3}
C113 0.369 0.866 0.634 ! 3.50 e A^{-3}
C114 0.625 0.313 0.418 ! 3.44 e A^{-3}
C115 0.579 0.631 0.459 ! 3.33 e A^{-3}
C116 0.540 0.908 0.208 ! 3.31 e A^{-3}
C117 0.653 0.291 0.962 ! 3.31 e A^{-3}
C118 0.345 0.079 0.483 ! 3.20 e A^{-3}
C119 0.047 0.150 0.049 ! 3.18 e A^{-3}
C120 0.173 0.580 0.155 ! 3.14 e A^{-3}
C121 0.750 0.398 0.002 ! 3.07 e A^{-3}
C122 0.226 0.013 0.202 ! 3.02 e A^{-3}
C123 0.514 0.703 0.724 ! 3.02 e A^{-3}
C124 0.048 0.498 0.157 ! 3.02 e A^{-3}
C125 0.970 0.023 0.282 ! 3.02 e A^{-3}

C126 0.468 0.532 0.227 ! 2.99 e A^{-3}
C127 0.968 0.032 0.727 ! 2.99 e A^{-3}
C128 0.775 0.976 0.094 ! 2.93 e A^{-3}
C129 0.625 0.314 0.432 ! 2.89 e A^{-3}
C130 0.394 0.297 0.443 ! 2.86 e A^{-3}
C131 0.395 0.695 0.117 ! 2.86 e A^{-3}
C132 0.394 0.180 0.430 ! 2.86 e A^{-3}
C133 0.718 0.049 0.387 ! 2.86 e A^{-3}
C134 0.695 0.889 0.126 ! 2.78 e A^{-3}
C135 1.002 0.672 0.416 ! 2.77 e A^{-3}
C136 1.000 0.115 0.225 ! 2.76 e A^{-3}
C137 0.728 0.882 0.274 ! 2.74 e A^{-3}
C138 0.023 0.656 0.466 ! 2.71 e A^{-3}
C139 0.080 0.070 0.398 ! 2.71 e A^{-3}
C140 0.952 0.203 0.133 ! 2.70 e A^{-3}
Q141 0.149 0.904 0.101 ! 2.69 e A^{-3}
C142 0.618 0.311 0.391 ! 2.67 e A^{-3}
C143 0.797 0.006 0.201 ! 2.67 e A^{-3}
C144 0.524 0.212 0.375 ! 2.66 e A^{-3}
C145 0.054 0.523 0.714 ! 2.65 e A^{-3}
C146 0.554 0.023 0.214 ! 2.65 e A^{-3}
C147 0.960 0.773 0.308 ! 2.64 e A^{-3}
C148 0.397 0.807 0.117 ! 2.64 e A^{-3}
C149 0.421 0.603 0.287 ! 2.62 e A^{-3}
C150 0.973 0.984 0.201 ! 2.62 e A^{-3}
Q151 0.720 0.253 0.033 ! 2.61 e A^{-3}
C152 0.975 0.663 0.303 ! 2.60 e A^{-3}
C153 0.135 0.137 0.073 ! 2.59 e A^{-3}
C154 0.398 0.726 0.294 ! 2.58 e A^{-3}
C155 0.672 0.805 0.116 ! 2.56 e A^{-3}
C156 0.007 0.728 0.426 ! 2.55 e A^{-3}
C157 0.174 0.476 0.762 ! 2.55 e A^{-3}
C158 0.578 0.717 0.297 ! 2.54 e A^{-3}
C159 0.626 0.215 0.406 ! 2.54 e A^{-3}
C160 0.259 0.323 0.738 ! 2.54 e A^{-3}
C161 0.759 0.823 0.238 ! 2.54 e A^{-3}
C162 0.380 0.168 0.449 ! 2.52 e A^{-3}
C163 0.880 0.668 0.949 ! 2.52 e A^{-3}

C164 0.203 0.539 0.000 ! 2.51 e A^{-3}
C165 0.995 0.429 0.996 ! 2.51 e A^{-3}
C166 0.816 0.243 0.761 ! 2.51 e A^{-3}
C167 0.376 0.341 0.227 ! 2.51 e A^{-3}
C168 0.844 0.728 0.873 ! 2.51 e A^{-3}
C169 0.775 0.072 0.218 ! 2.51 e A^{-3}
C170 0.970 0.822 0.523 ! 2.51 e A^{-3}
C171 0.539 0.283 0.072 ! 2.50 e A^{-3}
C172 0.366 0.926 0.023 ! 2.49 e A^{-3}
Q173 0.041 0.188 0.460 ! 2.48 e A^{-3}
C174 0.610 0.741 0.250 ! 2.47 e A^{-3}
C175 0.151 0.245 0.516 ! 2.46 e A^{-3}
C176 0.651 0.745 0.016 ! 2.46 e A^{-3}
C177 0.856 0.955 0.242 ! 2.45 e A^{-3}
C178 0.327 0.752 0.235 ! 2.45 e A^{-3}
C179 0.219 0.461 0.421 ! 2.45 e A^{-3}
C180 0.537 0.272 0.134 ! 2.44 e A^{-3}
C181 0.870 0.325 0.915 ! 2.43 e A^{-3}
C182 0.981 0.852 0.739 ! 2.43 e A^{-3}
C183 0.837 0.569 0.360 ! 2.43 e A^{-3}
C184 0.842 0.483 0.085 ! 2.43 e A^{-3}
Q185 0.373 0.075 0.108 ! 2.42 e A^{-3}
C186 0.984 0.077 0.229 ! 2.40 e A^{-3}
C187 0.375 0.655 0.237 ! 2.39 e A^{-3}
C188 0.112 0.039 0.489 ! 2.39 e A^{-3}
C189 0.205 0.633 0.146 ! 2.39 e A^{-3}
C190 1.001 0.647 0.407 ! 2.37 e A^{-3}
C191 0.523 0.259 0.296 ! 2.37 e A^{-3}
C192 0.813 0.100 0.432 ! 2.36 e A^{-3}
C193 0.625 0.702 0.172 ! 2.36 e A^{-3}
C194 0.187 0.109 0.023 ! 2.35 e A^{-3}
C195 0.619 0.318 0.321 ! 2.35 e A^{-3}
C196 0.913 0.330 0.008 ! 2.34 e A^{-3}
C197 0.572 0.737 0.273 ! 2.33 e A^{-3}
C198 0.880 0.455 0.271 ! 2.31 e A^{-3}
C199 0.380 0.955 0.771 ! 2.31 e A^{-3}

We estimated the number of the crystallization solvents according to the residual electron density in the solvent accessible void space, calculated from SQUEEZE routine (16227 electrons). We dissolved the reaction product in 4:1 ratio of H_2O/THF with SO_4^{2-} anions and crystallized **1**. Assuming that H_2O and THF are incorporated into the structure with 4:1 ratio and occupy the general position (48e), the estimated formula is $[Pt(en)(dpndi)]_4(SO_4)_4 \cdot 68H_2O \cdot 17THF$, corresponding to 16320 electrons (Table S1). This value is consistent with the calculated electron density in the solvent accessible void space of the unit cell (16227 electrons).

Table S1 Estimation of the solvent molecules in the solvent accessible voids of **1**.

Solvent	Number of electrons	Number of solvents	Total number of electrons
H_2O	10	68	8160
THF	40	17	8160

Considering the charge neutrality, elemental analysis and IR spectrum, four SO_4^{2-} should exist per square complex. In the crystallographic data, Pt occupies the Wyckoff position 48e, while the two SO_4^{2-} occupy the Wyckoff positions 24d (S1, O5 and O6) and 16c (S2, O7 and O8), respectively. This result is inconsistent with the charge neutrality. Although we tried many times, we could not find no more sites of SO_4^{2-} in the structural refinement. Therefore, the formula can be described as $[Pt(en)(dpndi)]_4(SO_4)_{3.333}[SO_4]_{0.667} \cdot 68H_2O \cdot 17THF$, to make it clear that 3.333 SO_4^{2-} were modelled and 0.667 SO_4^{2-} were not modelled.

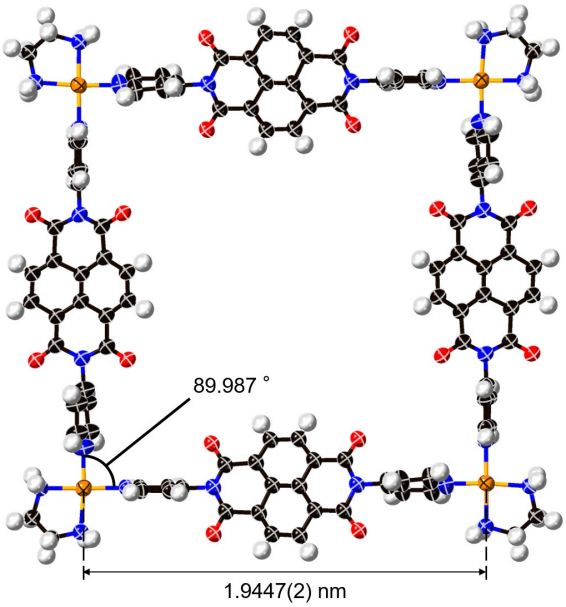

Fig. S9 Molecular structure of **1** at 100 K. The ellipsoids are drawn with a 50% probability (orange: Pt, red: O, blue: N, black: C, white: H). Counter anions are omitted for clarity.

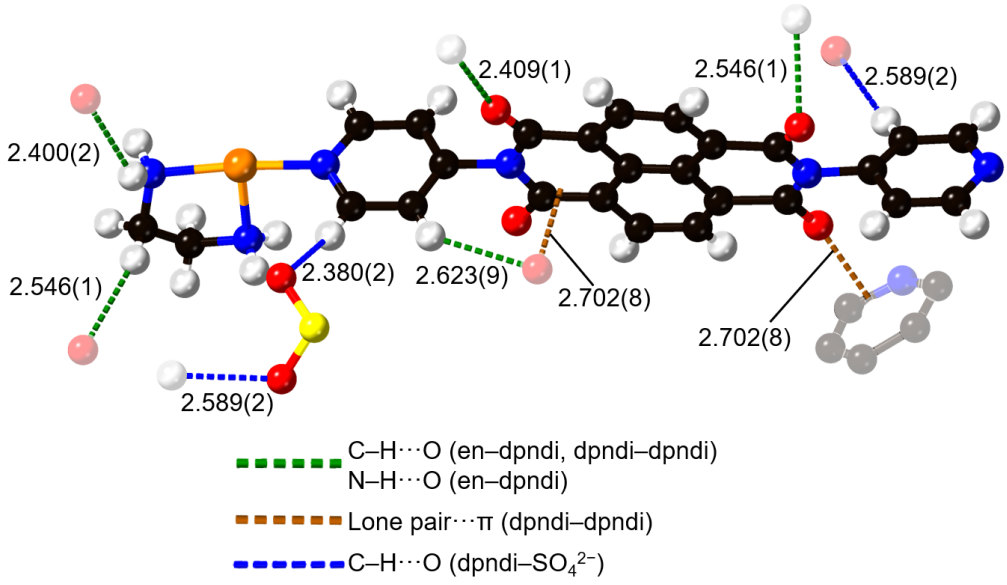

Fig. S10 Asymmetric unit of **1** (balls and solid line) and short contact atoms (shaded balls). Short contacts (Å) among the square units can be divided into three: C–H···O (en–dpndi and dpndi–dpndi) and N–H···O (en–dpndi) hydrogen bonding interactions (green dashed line), lone pair···π (dpndi–dpndi) interactions (brown dashed line) and C–H···O (dpndi–SO_4^{2-}) hydrogen bonding interactions (blue dashed line).

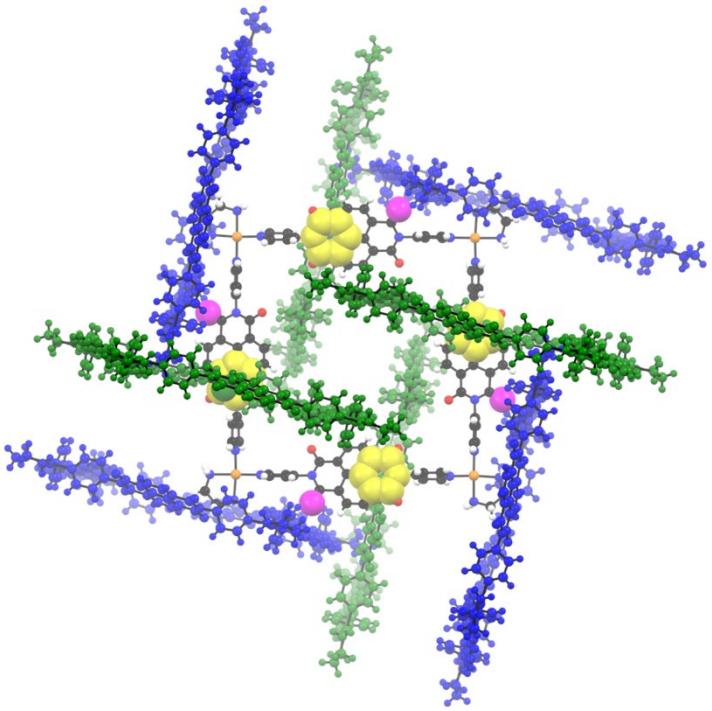

Fig. S11 Packing structure and interactions among the square units of **1**. The representation of the blue and green square units is the same as that in Fig. 7(a). The pink (yellow) moieties show the dominant interactions between the red and blue (green) square units, respectively.

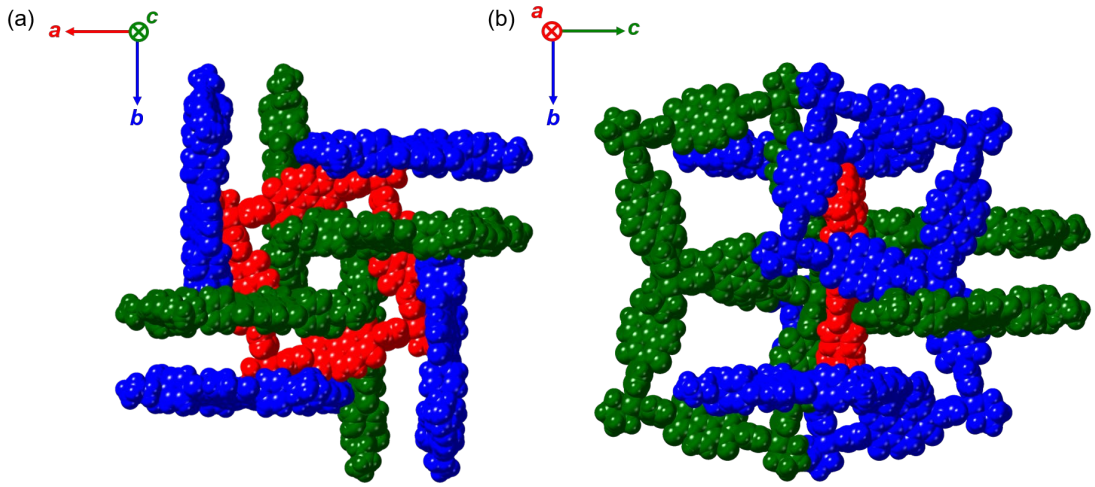

Fig. S12 Packing structure of the square units in **1** with 4-in–4-out manner from (a) the ***c***-axis and (b) the ***a***-axis. The representation of blue and green square units is the same as that in Fig. 7(a).

3. Calculation of Cavity Volume

The cavity space of **1** in the solid state was calculated using the 'Calculate > Cavities' command in CrystalMaker.[3] For the calculation, cavities among the square units and the counter anions were considered, and the radius of each atom was set to the van der Waals radius.[4] The minimum radius for searching the void space was set to 1.4 Å. The Wyckoff position, atomic coordinates, radius and volume of the calculated cavities are listed in Table S2. Also, the positions of the cavities among the square units are shown in Fig. S13–S17.

Table S2 List of Wyckoff position, atomic coordinates, radius and volume of the cavities for **1**.

	Wyckoff position	x	y	z	Radius / Å	Volume / Å^3
Cavity1	16c	0.8218	0.8218	0.8218	4.593	405.862
Cavity2	48e	0.2532	0.9620	0.0000	3.411	166.272
Cavity3	24d	0.1382	0.0000	0.2500	3.111	126.145
Cavity4	48e	0.5570	0.1266	0.8228	2.281	49.724
Cavity5	48e	0.5823	0.1139	0.9241	1.724	21.452
Cavity6	48e	0.5317	0.6582	0.7089	1.583	16.615
Cavity7	48e	0.7342	0.4430	0.7089	1.525	14.864
Cavity8	48e	0.3418	0.6203	0.5443	1.467	13.219
Cavity9	48e	0.4937	0.8734	0.4430	1.403	11.567

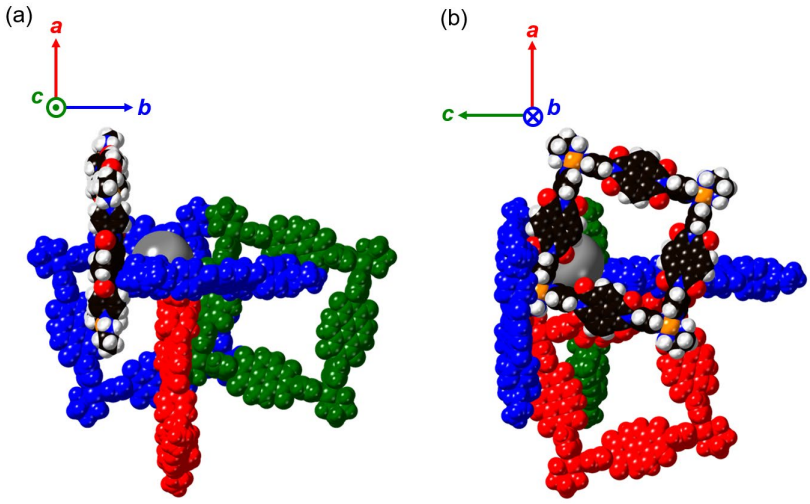

Fig. S13 (a) Position of the largest cavity (grey ball) in **1** and (b) 90° rotation of (a). Among the red, green, blue and the other square, a cavity with a radius of 4.59 Å exists.

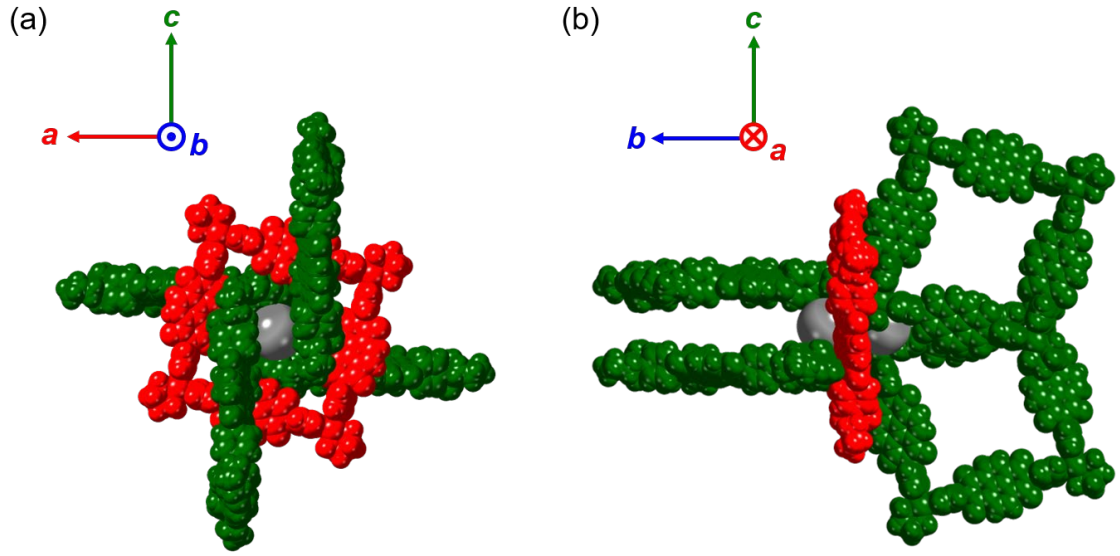

Fig. S14 (a) Position of the second-largest cavity (grey balls) in **1** and (b) 90° rotation of (a). Between the green and red squares, two cavities with a radius of 3.41 Å exist.

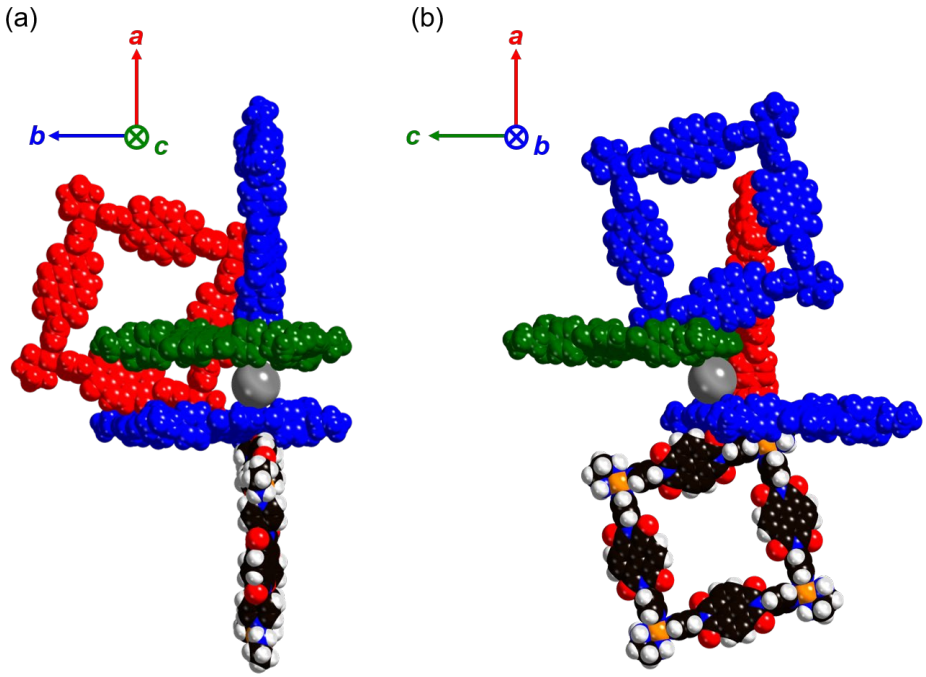

Fig. S15 (a) Position of the third-largest cavity (grey ball) in **1** and (b) 90° rotation of (a). Between the red, blue, green, and the other square, a cavity with a radius of 3.11 Å exists.

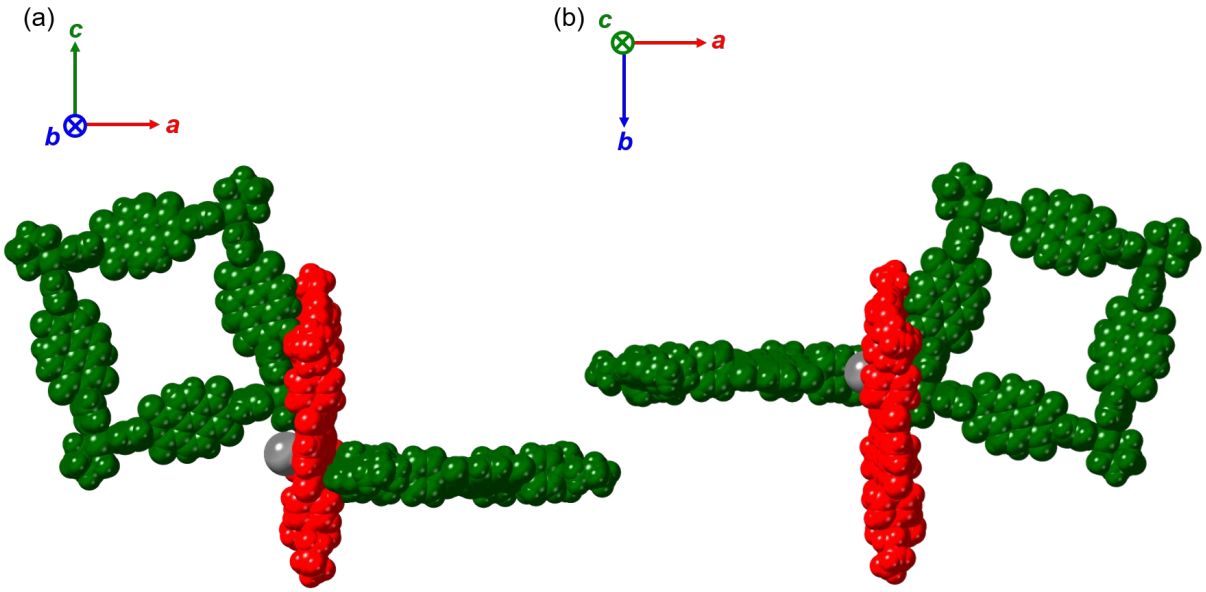

Fig. S16 (a) Position of the fourth-largest cavity (grey ball) in **1** and (b) 90° rotation of (a). Between the red and green squares, a cavity with a radius of 2.28 Å exist.

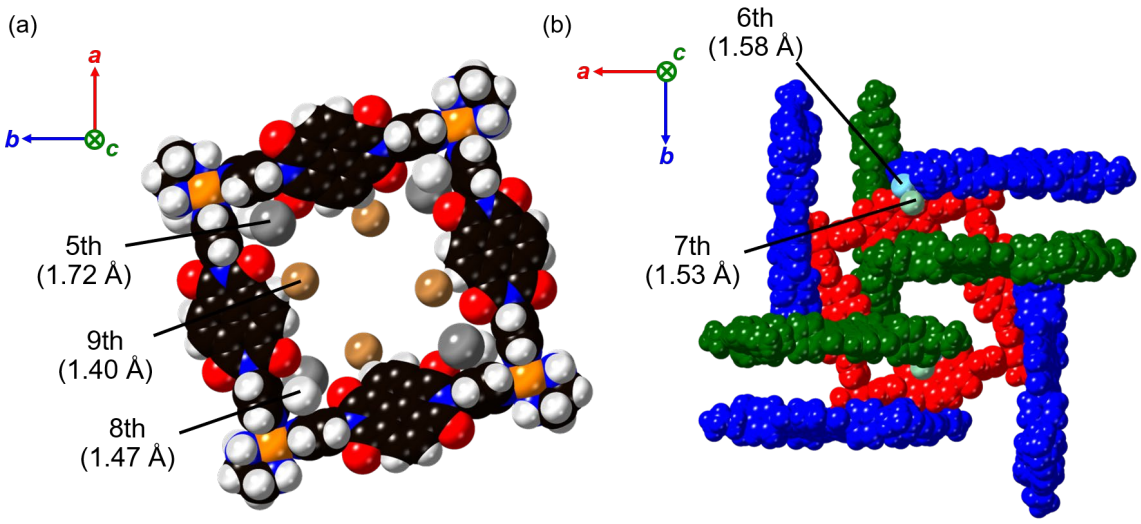

Fig. S17 (a) Position of the fifth- (grey, 1.72 Å), eighth- (white, 1.47 Å) and ninth (brown, 1.40 Å) largest cavities in **1**. (b) Sixth- (green, 1.58 Å) and seventh- (light blue, 1.53 Å) largest cavities in **1**.

4. Theoretical Calculation Result.

Table S3 Atomic coordinates of the optimized structure of dpndi.

	Coordinates / Angstroms				Coordinates / Angstroms		
Element	x	y	z	Element	x	y	z
C	−0.7081230	0.0000000	−0.0000030	C	0.7081230	0.0000000	0.0000010
N	−3.5704260	0.0000010	−0.0000060	N	3.5704260	−0.0000010	0.0000050
C	−1.4062760	−1.2350630	−0.1588780	C	1.4062760	1.2350640	0.1588760
O	−3.5410250	2.2857370	0.2512210	O	3.5410250	−2.2857370	−0.2512210
C	−1.4062760	1.2350640	0.1588690	C	1.4062760	−1.2350640	−0.1588710
O	−3.5410250	−2.2857370	−0.2512250	O	3.5410250	2.2857370	0.2512240
C	−2.8997100	1.2649590	0.1467470	C	2.8997100	−1.2649590	−0.1467500
C	−2.8997100	−1.2649580	−0.1467620	C	2.8997100	1.2649580	0.1467620
C	−0.7118650	−2.4159090	−0.3184090	C	0.7118650	2.4159090	0.3184080
H	−1.2511060	−3.3642970	−0.4438540	H	1.2511060	3.3642970	0.4438530
N	−7.8356520	−0.0000010	0.0000080	N	7.8356510	0.0000010	−0.0000030
C	−0.7118660	2.4159090	0.3184050	C	0.7118660	−2.4159090	−0.3184070
H	−1.2511070	3.3642980	0.4438480	H	1.2511070	−3.3642980	−0.4438490
C	−5.0330330	0.0000000	−0.0000020	C	5.0330320	0.0000000	0.0000020
C	−5.7332020	0.8874100	−0.8299820	C	5.7332010	−0.8874110	0.8299820
H	−5.2133480	1.6009060	−1.4672010	H	5.2133460	−1.6009070	1.4672000
C	−7.1363370	0.8531650	−0.7925410	C	7.1363360	−0.8531660	0.7925440
H	−7.7327570	1.5298780	−1.4174770	H	7.7327550	−1.5298800	1.4174800
C	−5.7331960	−0.8874110	0.8299830	C	5.7331970	0.8874110	−0.8299810
H	−5.2133370	−1.6009060	1.4671990	H	5.2133390	1.6009070	−1.4671970
C	−7.1363310	−0.8531670	0.7925520	C	7.1363320	0.8531680	−0.7925480
H	−7.7327460	−1.5298800	1.4174920	H	7.7327480	1.5298810	−1.4174860
C	−0.7081230	0.0000000	−0.0000030	C	0.7081230	0.0000000	0.0000010

Table S4 Atomic coordinates of the optimized structure of square unit of **1**.

	Coordinates / Angstroms				Coordinates / Angstroms		
Element	x	y	z	Element	x	y	z
N	11.869688	−9.935121	0.147338	C	−9.073678	7.061115	0.952102
N	9.935251	11.869728	0.145111	C	−7.061227	−9.073993	0.950991
N	−11.869688	9.935121	0.147338	C	10.555124	−7.059844	−0.852518
N	−9.935251	−11.869728	0.145111	C	7.061227	9.073993	0.950991
N	9.935251	−11.869702	−0.145777	C	−10.555124	7.059844	−0.852518
N	11.869676	9.935111	−0.147838	C	−5.676514	−9.062261	0.978206
N	−9.935251	11.869702	−0.145777	C	10.602361	−5.678083	−0.859818
N	−11.869676	−9.935111	−0.147838	C	5.676514	9.062261	0.978206
N	7.758484	−9.808344	−0.044996	C	−10.602361	5.678083	−0.859818
N	9.808228	7.758486	−0.046208	C	−4.954294	−9.839509	0.064631
N	−7.758484	9.808344	−0.044996	C	9.839305	−4.954290	0.065577
N	−9.808228	−7.758486	−0.046208	C	4.954294	9.839509	0.064631
N	3.531858	−9.845117	−0.061830	C	−9.839305	4.954290	0.065577
N	9.844905	3.531852	−0.062174	C	−12.317157	11.325411	−0.287523
N	−3.531858	9.845117	−0.061830	H	−9.222207	−12.368871	−0.404707
N	−9.844905	−3.531852	−0.062174	Pt	9.802328	−9.802337	0.000694
N	−3.531867	−9.845159	0.061912	Pt	9.802328	9.802340	−0.001003
N	9.844944	−3.531863	0.062665	Pt	−9.802328	9.802337	0.000694
N	3.531867	9.845159	0.061912	Pt	−9.802328	−9.802340	−0.001003
N	−9.844944	3.531863	0.062665	O	3.507860	−7.540856	−0.236992
N	−7.758490	−9.808374	0.044844	O	7.540659	3.507816	−0.237548
N	9.808255	−7.758493	0.046203	O	−3.507860	7.540856	−0.236992
N	7.758490	9.808374	0.044844	O	−7.540659	−3.507816	−0.237548
N	−9.808255	7.758493	0.046203	O	−3.507884	−7.540956	0.237846
C	12.317157	−11.325411	−0.287523	O	7.540713	−3.507852	0.238276
C	11.325491	12.317011	−0.290100	O	3.507884	7.540956	0.237846
C	−11.325491	−12.317011	−0.290100	O	−7.540713	3.507852	0.238276
C	11.325532	−12.317049	0.289238	O	−3.529801	−12.149035	−0.117803
C	12.317172	11.325480	0.286745	O	12.148845	−3.529809	−0.116759
C	−11.325532	12.317049	0.289238	O	3.529801	12.149035	−0.117803
C	−12.317172	−11.325480	0.286745	O	−12.148845	3.529809	−0.116759
C	7.061164	−9.073688	−0.950876	O	3.529813	−12.149051	0.117126

C	10.555166	7.059942	0.852537	O	12.148827	3.529829	0.116983
C	−7.061164	9.073688	−0.950876	O	−3.529813	12.149051	0.117126
C	−10.555166	−7.059942	0.852537	O	−12.148827	−3.529829	0.116983
C	5.676451	−9.061937	−0.977998	H	12.368923	−9.222143	−0.402481
C	10.602397	5.678182	0.860003	H	9.783477	12.129149	1.133163
C	−5.676451	9.061937	−0.977998	H	−9.783477	−12.129149	1.133163
C	−10.602397	−5.678182	0.860003	H	12.128858	−9.783162	1.135427
C	4.954284	−9.839461	−0.064617	H	9.222207	12.368871	−0.404707
C	9.839259	4.954279	−0.065236	H	5.171844	−8.445339	−1.705776
C	−4.954284	9.839461	−0.064617	H	9.222261	−12.368946	0.404018
C	−9.839259	−4.954279	−0.065236	H	12.128766	9.782983	−1.135923
C	5.678012	−10.602606	0.860751	H	−9.222261	12.368946	0.404018
C	9.061770	5.676278	−0.978781	H	−12.128766	−9.782983	−1.135923
C	−5.678012	10.602606	0.860751	H	9.783394	−12.128956	−1.133860
C	−9.061770	−5.676278	−0.978781	H	12.368966	9.222234	0.402062
C	7.059772	−10.555327	0.853581	H	−9.783394	12.128956	−1.133860
C	9.073561	7.060997	−0.951949	H	−12.368966	−9.222234	0.402062
C	−7.059772	10.555327	0.853581	H	12.309283	−11.345762	−1.381548
C	−9.073561	−7.060997	−0.951949	H	11.526975	13.332826	0.064841
C	2.867239	−8.587141	−0.130500	H	−11.526975	−13.332826	0.064841
C	8.586936	2.867219	−0.130840	H	13.332893	−11.526780	0.067712
C	−2.867239	8.587141	−0.130500	H	11.345653	12.308857	−1.384128
C	−8.586936	−2.867219	−0.130840	H	−11.345653	−12.308857	−1.384128
C	1.396567	−8.626168	−0.052291	H	11.345789	−12.309081	1.383264
C	8.625958	1.396558	−0.052410	H	13.332876	11.526794	−0.068611
C	−1.396567	8.626168	−0.052291	H	−13.332876	−11.526794	−0.068611
C	−8.625958	−1.396558	−0.052410	H	11.526993	−13.332802	−0.065895
C	0.701499	−7.430968	−0.034409	H	12.309391	11.346019	1.380768
C	7.430757	0.701490	−0.034558	H	−11.526993	13.332802	−0.065895
C	−0.701499	7.430968	−0.034409	H	−12.309391	−11.346019	1.380768
C	−7.430757	−0.701490	−0.034558	H	7.635906	−8.494193	−1.661278
C	−0.701522	−7.430984	0.035360	H	11.099862	7.628842	1.595971
C	7.430768	−0.701522	0.035413	H	−7.635906	8.494193	−1.661278
C	0.701522	7.430984	0.035360	H	−11.099862	−7.628842	1.595971
C	−7.430768	0.701522	0.035413	H	11.229447	5.177657	1.582357
C	−1.396582	−8.626195	0.052831	H	−5.171844	8.445339	−1.705776

C	8.625977	−1.396578	0.053126	H	−11.229447	−5.177657	1.582357
C	1.396582	8.626195	0.052831	H	5.177351	−11.229683	1.582987
C	−8.625977	1.396578	0.053126	H	8.445173	5.171538	−1.706467
C	−2.867256	−8.587203	0.131021	H	−5.177351	11.229683	1.582987
C	8.586977	−2.867241	0.131517	H	−8.445173	−5.171538	−1.706467
C	2.867256	8.587203	0.131021	H	7.628529	−11.100014	1.597131
C	−8.586977	2.867241	0.131517	H	8.494095	7.635607	−1.662481
C	−2.873106	−11.114842	−0.026517	H	−7.628529	11.100014	1.597131
C	11.114637	−2.873108	−0.025673	H	−8.494095	−7.635607	−1.662481
C	2.873106	11.114842	−0.026517	H	1.260104	−6.503173	−0.070223
C	−11.114637	2.873108	−0.025673	H	6.502965	1.260087	−0.070558
C	−1.400056	−11.084500	0.002632	H	−1.260104	6.503173	−0.070223
C	11.084287	−1.400054	0.003224	H	−6.502965	−1.260087	−0.070558
C	1.400056	11.084500	0.002632	H	−1.260132	−6.503205	0.071490
C	−11.084287	1.400054	0.003224	H	6.502985	−1.260128	0.071515
C	−0.704306	−12.279314	−0.007591	H	1.260132	6.503205	0.071490
C	12.279101	−0.704304	−0.006976	H	−6.502985	1.260128	0.071515
C	0.704306	12.279314	−0.007591	H	−1.257899	−13.211461	−0.021880
C	−12.279101	0.704304	−0.006976	H	13.211250	−1.257898	−0.021064
C	0.704315	−12.279312	0.006920	H	1.257899	13.211461	−0.021880
C	12.279095	0.704320	0.007297	H	−13.211250	1.257898	−0.021064
C	−0.704315	12.279312	0.006920	H	1.257915	−13.211460	0.020899
C	−12.279095	−0.704320	0.007297	H	13.211240	1.257923	0.021280
C	1.400058	−11.084490	−0.002910	H	−1.257915	13.211460	0.020899
C	11.084273	1.400059	−0.002776	H	−13.211240	−1.257923	0.021280
C	−1.400058	11.084490	−0.002910	H	−5.177266	−11.229242	−1.583400
C	−11.084273	−1.400059	−0.002776	H	8.445378	−5.171746	1.706919
C	2.873108	−11.114832	0.026208	H	5.177266	11.229242	−1.583400
C	11.114612	2.873113	0.026085	H	−8.445378	5.171746	1.706919
C	−2.873108	11.114832	0.026208	H	−7.628446	−11.099576	−1.597643
C	−11.114612	−2.873113	0.026085	H	8.494273	−7.635814	1.662613
C	0.708449	−9.855363	−0.014091	H	7.628446	11.099576	−1.597643
C	9.855148	0.708447	−0.013974	H	−8.494273	7.635814	1.662613
C	−0.708449	9.855363	−0.014091	H	−7.636014	−8.494706	1.661526
C	−9.855148	−0.708447	−0.013974	H	11.099762	−7.628658	−1.596061
C	−0.708456	−9.855372	0.014225	H	7.636014	8.494706	1.661526

C	9.855157	−0.708454	0.014563	H	−11.099762	7.628658	−1.596061
C	0.708456	9.855372	0.014225	H	−5.171950	−8.445888	1.706204
C	−9.855157	0.708454	0.014563	H	11.229350	−5.177473	−1.582164
C	−5.677968	−10.602377	−0.861009	H	5.171950	8.445888	1.706204
C	9.061902	−5.676399	0.979110	H	−11.229350	5.177473	−1.582164
C	5.677968	10.602377	−0.861009	H	−11.345789	12.309081	1.383264
C	−9.061902	5.676399	0.979110	H	−12.309283	11.345762	−1.381548
C	−7.059728	−10.555100	−0.853908	H	−13.332893	11.526780	0.067712
C	9.073678	−7.061115	0.952102	H	−12.368923	9.222143	−0.402481
C	7.059728	10.555100	−0.853908	H	−12.128858	9.783162	1.135427

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