Supporting Information

Wavelength-Dependent Tri-State Photoswitching in Crystals via Synergistic Dimer Confinement and Charge-Transfer Stacking

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Materials and Methods

The ligand N,N'-bis(5-isophthalic acid) naphthalenediimide (H_4BINDI) was synthesized according to the literature[1]. 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride was purchased from TCI chemicals. Hydrochloric acid and Na_2SO_4 were purchased from Tianjin Bohua Chemical Reagent. 5-aminoisophthalic acid was purchased from Bide Pharmatech. Anthracene was purchased from HEOWNS. 2,2,6,6-tetramethylpiperidine(TEMP), $Ca(NO_3)_2$•$4H_2O$, and $Sr(NO_3)_2$ were purchased from Shanghai Aladdin Biochemical Technology. Ethanol (EtOH) was purchased from Tianjin Guangshunda Chemical Reagent. Dimethylformamide (DMF) was purchased from Tianjin Huixiang Chemical Technology.

All of the above-mentioned chemicals were used as received without further purification.

Thermogravimetric analysis (TGA) was carried out at a ramp rate of 10 °C/min in a nitrogen flow using a NETZSCH TG 209 F3 Tarsus®. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker AVANCEIII 400 MHz spectrometer (DMSO-d_6 as solvent, δ = 2.50 ppm; TMS as standard, δ = 0.00 ppm). Photoluminescence spectra were measured on an Edinburgh FLS1000 spectrometer. UV–vis absorption spectra were recorded on a GENESYS 180 UV–visible Spectrophotometer. The lasers used in all tests were 635 nm and 808 nm solid-state lasers (Changchun New Industries Optoelectronics Tech., China).

Syntheses of MOFs

Synthesis of Sr-NDI: Sr-NDI was synthesized based on literature[1].

Synthesis of Sr-NDI@An: H_4BINDI(21 mg), $Sr(NO_3)_2$ (24 mg), anthracene (18 mg), 0.3 mL HCl (3 M) and 2.0 mL DMF were mixed and stirred for 2 h at room temperature and then transferred to a 5 mL glass vial and heated at 100 °C for 36 h. After the mixture was slowly cooled to room temperature, light-purple rod crystals were obtained for single crystal X-ray diffraction.

Synthesis of Ca-NDI@An: H_4BINDI(21 mg), $Ca(NO_3)_2 \cdot 4H_2O$(24 mg), anthracene (14 mg), 0.3 mL HCl (3 M) and 2.0 mL DMF were mixed and stirred for 2 h at room temperature and then transferred to a 5 mL glass vial and heated at 100 °C for 36 h. After the mixture was slowly cooled to room temperature, orange red crystals were obtained for single crystal X-ray diffraction.

Single Crystal X-ray Crystallography of Sr-NDI@An and Ca-NDI@An

Intensities were collected on a XtaLAB Synergy-R (Rigaku oxford diffraction) with graphite monochromated CuK\a (l= 1.54178 Å) using the SMART[2] SAINT[3] programs. The structure was solved by direct methods and refined on F^2 with the SHELX-2018[4] and Olex2[5] oftware package. Non-hydrogen atoms of the ligand backbones were refined anisotropically. Hydrogen atoms within the ligand backbones were fixed geometrically at calculated positions and allowed to ride on the parent non-hydrogen atoms. To assist the stability of refinements, partial DMF solvent molecules were restrained as idealized regular polygons and thermal parameters on adjacent atoms in DMF molecules were restrained to be similar. partial DMF solvent molecules were disordered into two parts with the *s.o.f* of each part being fixed at free values. The SQUEEZE subroutine in PLATON was used. Hydrogen atoms of the solvent molecules were found from the different Fourier MAP, but refined

using the riding model with the thermal parameter being fixed at 1.2 times of the oxygen atoms they attached.

Supplementary Experimental Methods of Electrochemical testing

The Electrochemical impedance experiment and the photocurrent experiments were measured using CHI760E Electrochemical Workstation with a typical three-electrode system. The sample mounted on ITO served as the working electrode. 5 mg MOF power was well dispersed with 50 μL Nafion and 500 μL DMA. After mounting the sample onto the ITO, the composite photocathode was left to dry naturally. A platinum wire and $Ag/AgNO_3$ electrode served as the counter and reference electrodes, respectively. The electrolyte used in the electrochemical tests was a 1.0 M Na_2SO_4 solution in H_2O. A 450 nm LED lamp (30 W) was used as the light source during the photocurrent experiments.

Supplementary Experimental Methods of the solid-state UV-visible absorption spectra

The MOF cocrystals and $BaSO_4$ powder are mixed in a mass ratio of 1:1, thoroughly combined, then pressed into a transparent sheet, and placed on the UV-Visible/NIR spectrophotometer (Thermo Fisher Scientific Evolution 220) to measure the solid UV-vis absorption spectra.

Supplementary Experimental Methods of the [4+4] cycloaddition reaction of Sr-NDI@An and Ca-NDI@An under UV light irradiation

5 mg single crystal was irradiated by a xenon lamp with 365 nm optical filter (CEL-HXF300-T3, CEAULIGHT, China) from a distance of 5 cm for various periods. Following the irradiation, 20 μL of D_2SO_4 and 500 μL of DMSO-d_6 were added to the crystal for ^{1}H nuclear magnetic resonance (^{1}H NMR) spectral analysis. The crystals after irradiation at 365 nm for 4 h were heated in an oven at 120 ℃ for 2 h to undergo the reverse cycloaddition reaction, and 20 μL D_2SO_4 and 500 μL DMSO-d_6 were added to the crystals for ^{1}H NMR spectral analysis.

Supplementary Experimental Methods of the [4+2] cycloaddition reaction of Sr-NDI@An under 635 nm light irradiation

5 mg single crystal was irradiated by a 635 nm laser from a distance of 27 cm for various periods. Following the irradiation, 20 μL of D_2SO_4 and 500 μL of DMSO-d_6 were added to the crystal for ^{1}H NMR spectral analysis.

Electron paramagnetic resonance (EPR) measurements

To investigate the generation of long-lived radical species in Sr-NDI@An under 808 nm laser irradiation, the experimental procedure was conducted as follows: First, 10 mg of the crystal was placed in an NMR tube and irradiated with 808 nm laser under ambient conditions, followed by EPR measurements（Bruker EPR spectrometer E580-10/12）. Additionally, two supplementary tests were performed: (1) measurement after leaving the sample uncapped for 5 days, and (2) measurement after both uncapping for 5 days and

subsequently purging the tube with oxygen.

To confirm the generation of $^1O_2$ by Sr-NDI@An under 635 nm light irradiation, 20 mg of the crystal was added to a TEMP (2,2,6,6-tetramethylpiperidine)/toluene solution (60 μL/9 mL). After irradiation with 635 nm light at room temperature for a certain period, 500 μL of the mixture was transferred into an NMR tube, and EPR spectroscopy was performed under ambient conditions.

Theoretical Calculations

The geometric structure of Sr-NDI@An required for the calculations was obtained from single-crystal diffraction data. Restricted optimization (optimizing only H atoms) of the complex was carried out using the PM6-D3H4 method. The single-point energy and molecular orbital calculations conducted via the DFT B3LYP-D3(BJ)/def2-sv(p) method. The calculations were carried out using MOPAC and ORCA 6.0.

Table S1. Crystallographic data for Sr-NDI, Sr-NDI@An and Ca-NDI@An

Compound	Sr-NDI[1]	Sr-NDI@An	Ca-NDI@An
Empirical formula	$C_{44}H_{44}Sr_2N_4O_{23}$	$C_{56}H_{48}Sr_2N_6O_{16}$	$C_{89}H_{71.67}Ca_4N_9O_{29.48}$
Formula wt	1172.07	1236.24	1899.24
T/K	200.01(2)	293(2)	293(2)
Crystal system	Tetragonal	Tetragonal	Monoclinic
Space group	*I* 41/a	*I* 41/a	*C 2/c*
a/Å	28.4784(4)	28.42240(10)	41.8161(5)
b/Å	28.4784(4)	28.42240(10)	10.36690(10)
c/Å	13.6334(3)	13.71600(10)	24.5777(3)
β/deg	90.00	90.00	125.5490(10)
V/Å^3	11056.9(5)	11080.24(11)	8668.71(19)
Z	8	8	4
D_{calcd}/g	1.408	1.482	1.455
μ/mm^{-1}	2.008	3.175	2.942
No. of rflns collected	11940	77236	27344
No. of unique rflns	6341	5796	7599
R(int)	0.0447	0.0622	0.0333
F(000)	4768	5040	3938
R1 ($I>2\sigma$)[a]	0.1393	0.0665	0.0787
R1 (all data)[a]	0.1810	0.0672	0.0844
wR2 ($I>2\sigma$)[b]	0.3624	0.1910	0.2293
wR2 (all data)[b]	0.3919	0.1919	0.2374
GOF	0.930	1.083	1.045
CCDC No.	1412539	2419043	2418888

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = |\sum w(|F_o|^2 - |F_c|^2)|/\sum|w(F_o^2)^2|^{1/2}$

Table S2. Bond lengths of Sr-O cluster of Sr-NDI and Sr-NDI@An

Bond type	Sr-NDI	Sr-NDI@An
Sr- bidentate carboxylic groups	2.55 Å -2.72 Å	2.54 Å – 2.73 Å
Sr-monodentate carboxylic groups	2.48 Å - 2.51 Å	2.50 Å – 2.52 Å
Sr-DMF	2.55 Å, 2.59 Å	2.55 Å, 2.58 Å

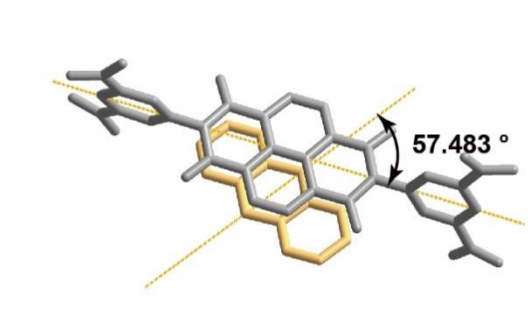
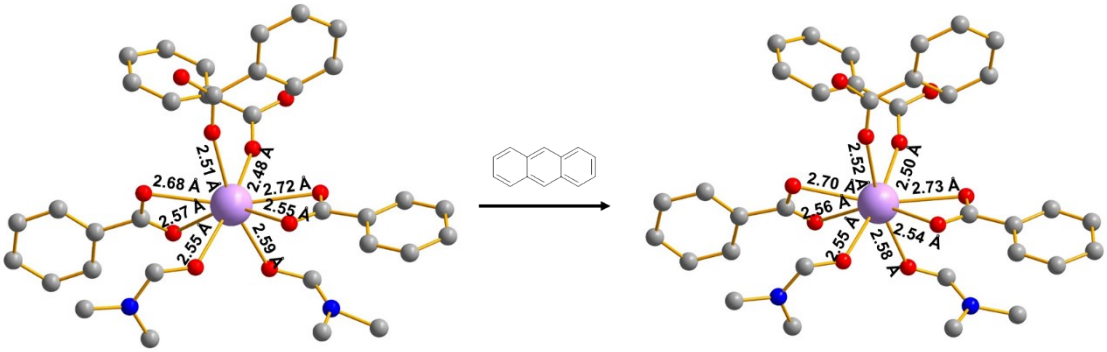


Figure S1. The dihedral angle between the transition dipoles of NDI and An.



Sr-NDI Sr-NDI@An

Figure S2. Schematic illustration of the An-encapsulation induced changes in the coordination environment of Sr^{2+} for Sr-NDI. The bond lengths of metal-oxygen bonds are marked.

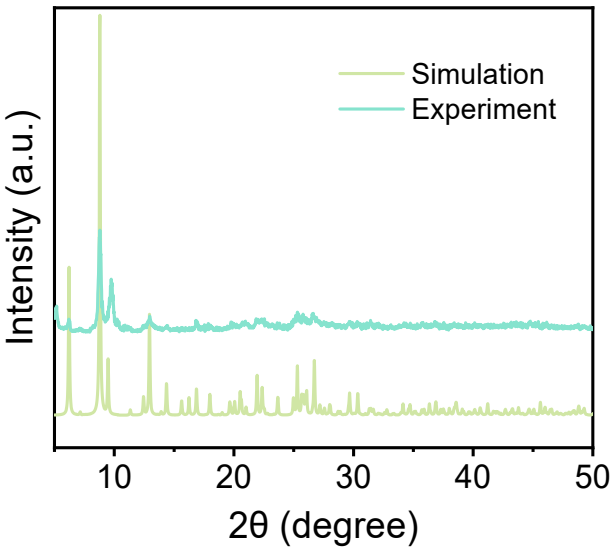


Figure S3. PXRD patterns of Sr-NDI@An.

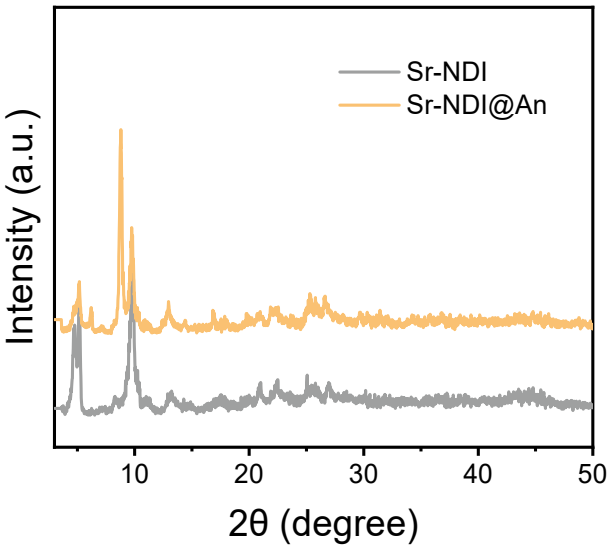


Figure S4. PXRD patterns of Sr-NDI and Sr-NDI@An.

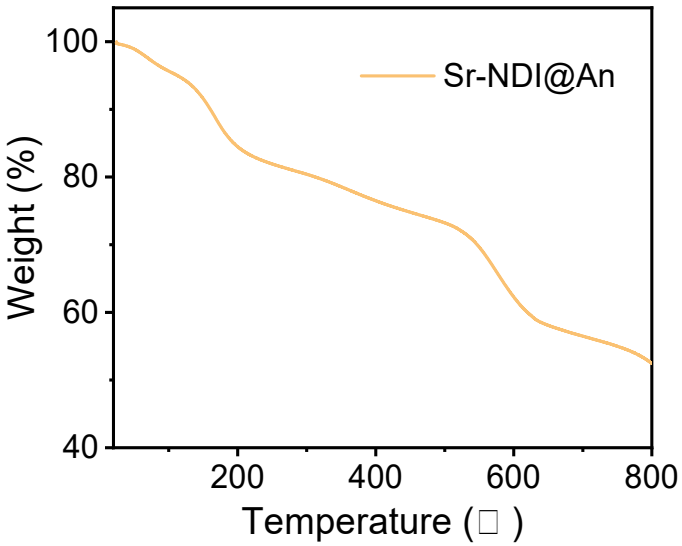


Figure S5. Thermogravimetric figure of Sr-NDI@An.

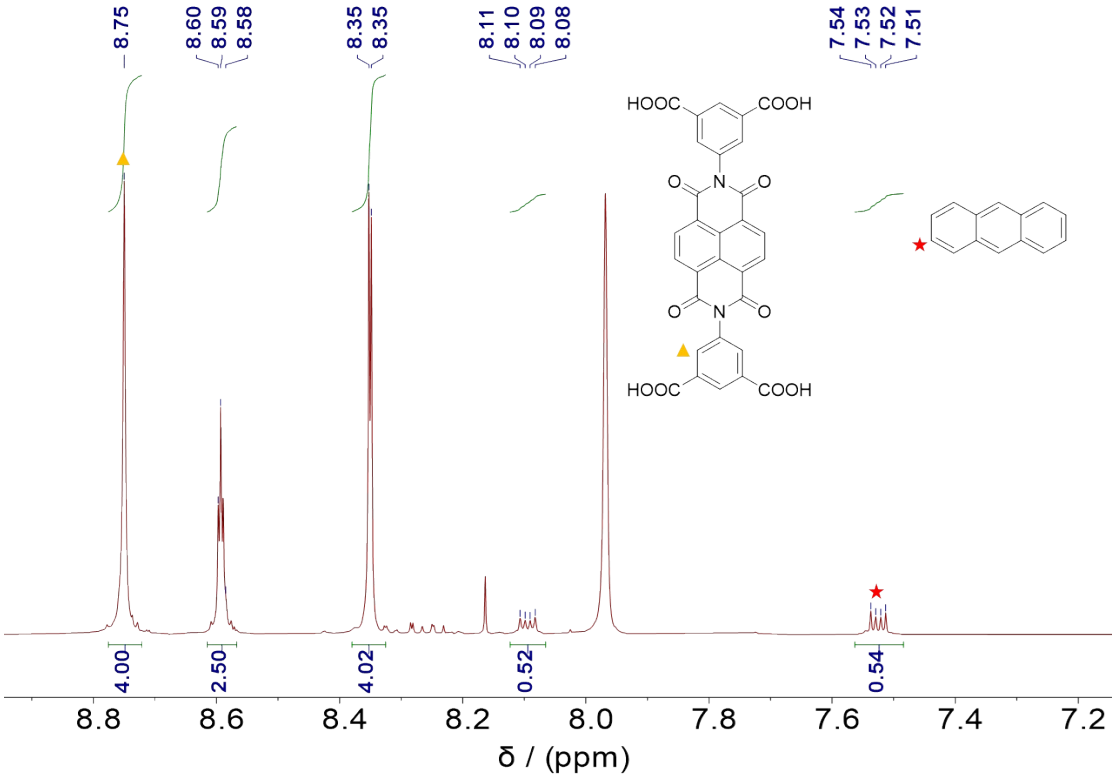


Figure S6. Partial ^{1}H NMR spectrum of Sr-NDI@An in D_2SO_4/DMSO-d_6.

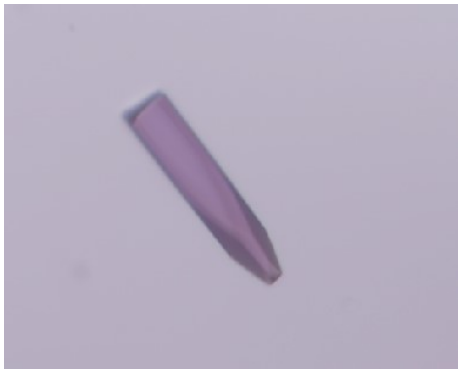


Figure S7. Picture of Sr-NDI@An crystal.

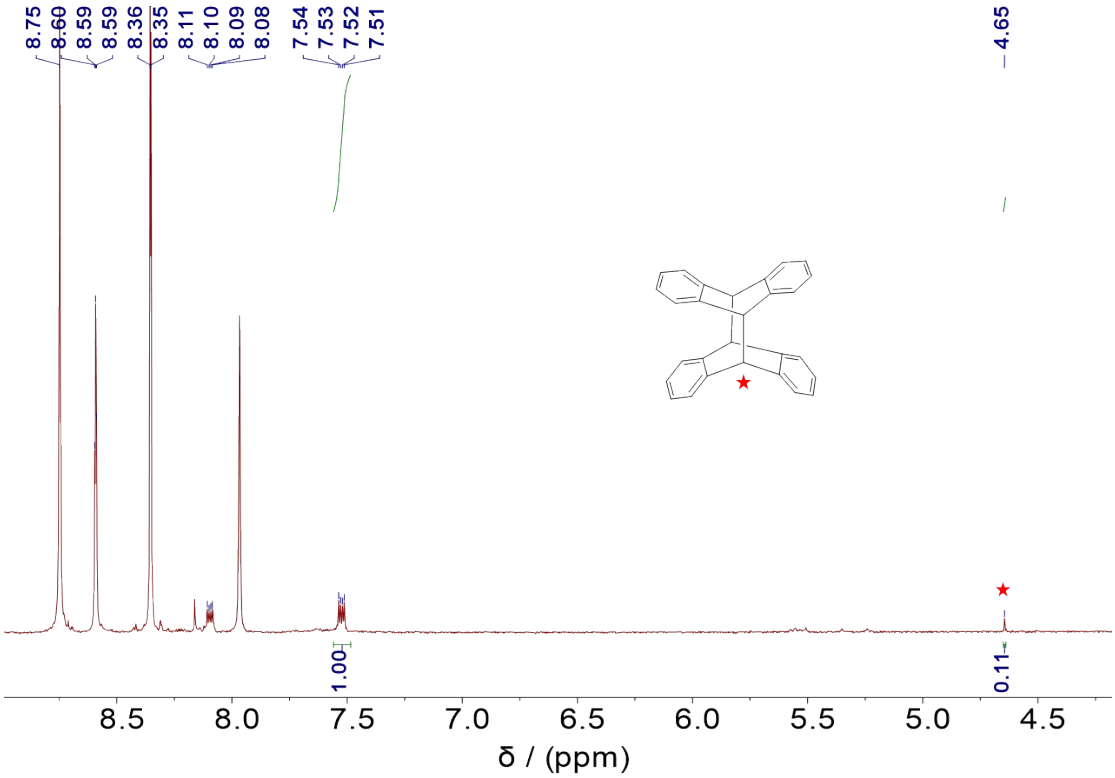


Figure S8. Partial ^{1}H NMR spectrum of Sr-NDI@An in D_2SO_4/DMSO-d_6 after UV illumination for 20 min.

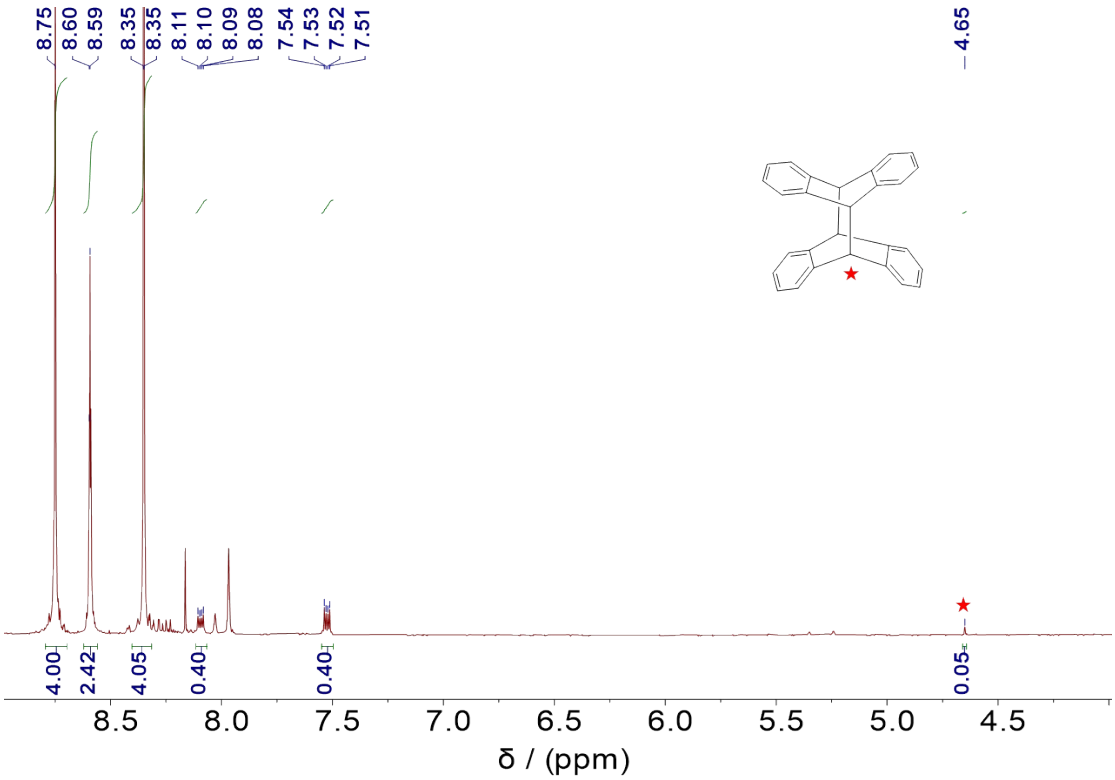


Figure S9. Partial ^{1}H NMR spectrum of the 4 hours UV-irradiated Sr-NDI@An in D_2SO_4/DMSO-d_6 after heating at 120 ℃ for 2 hours.

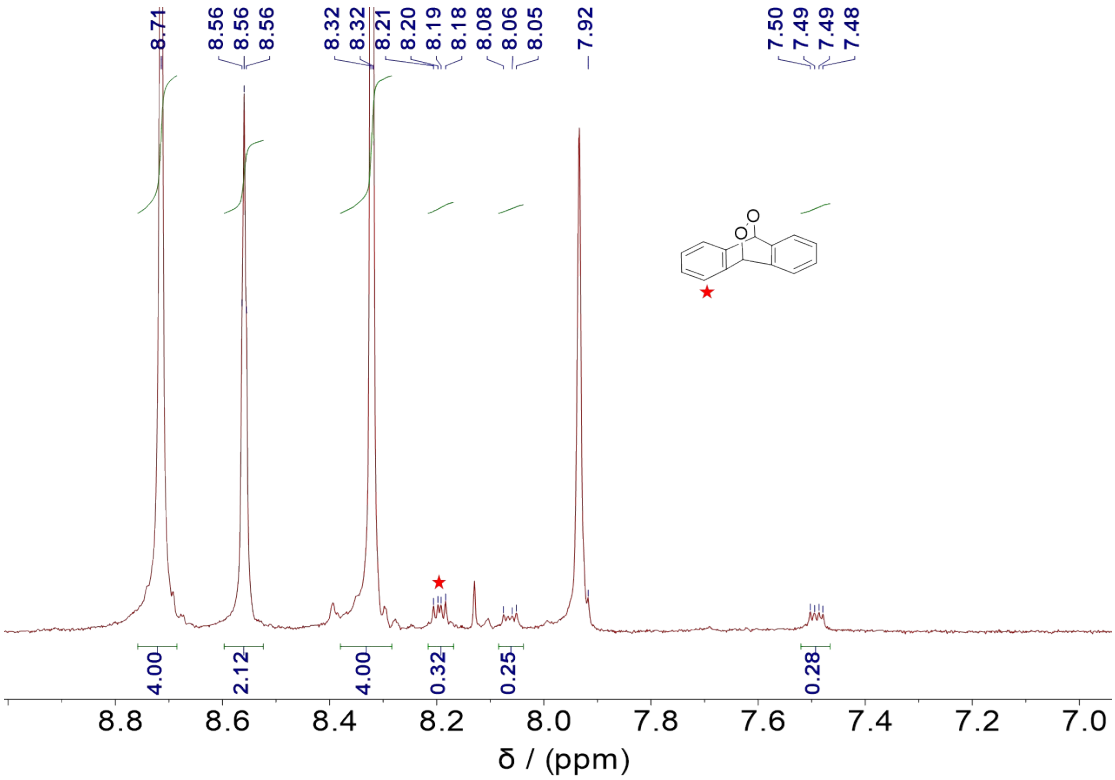


Figure S10. Partial ^{1}H NMR spectrum of Sr-NDI@An in D_2SO_4/DMSO-d_6 after 2 hours of illumination at 635 nm.

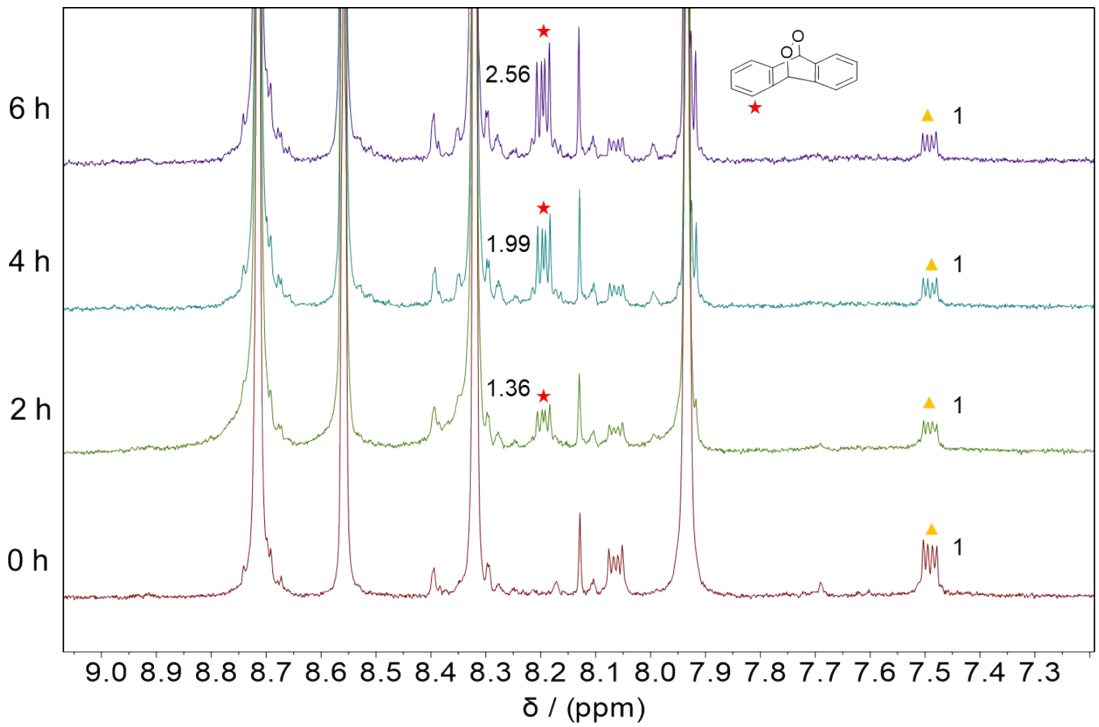


Figure S11. ^{1}H NMR monitoring of the hetero-Diels-Alder reaction of Sr-NDI@An with illumination at 635 nm.

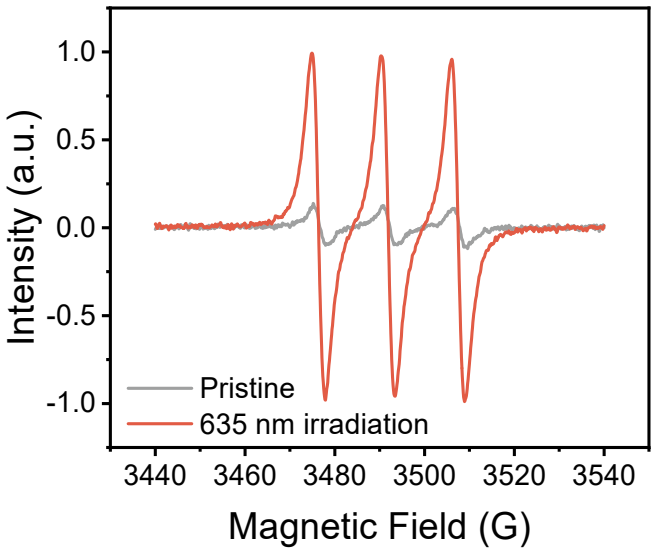


Figure S12. Electron paramagnetic resonance (EPR) spectra of Sr-NDI@An before and after 635 nm illumination.

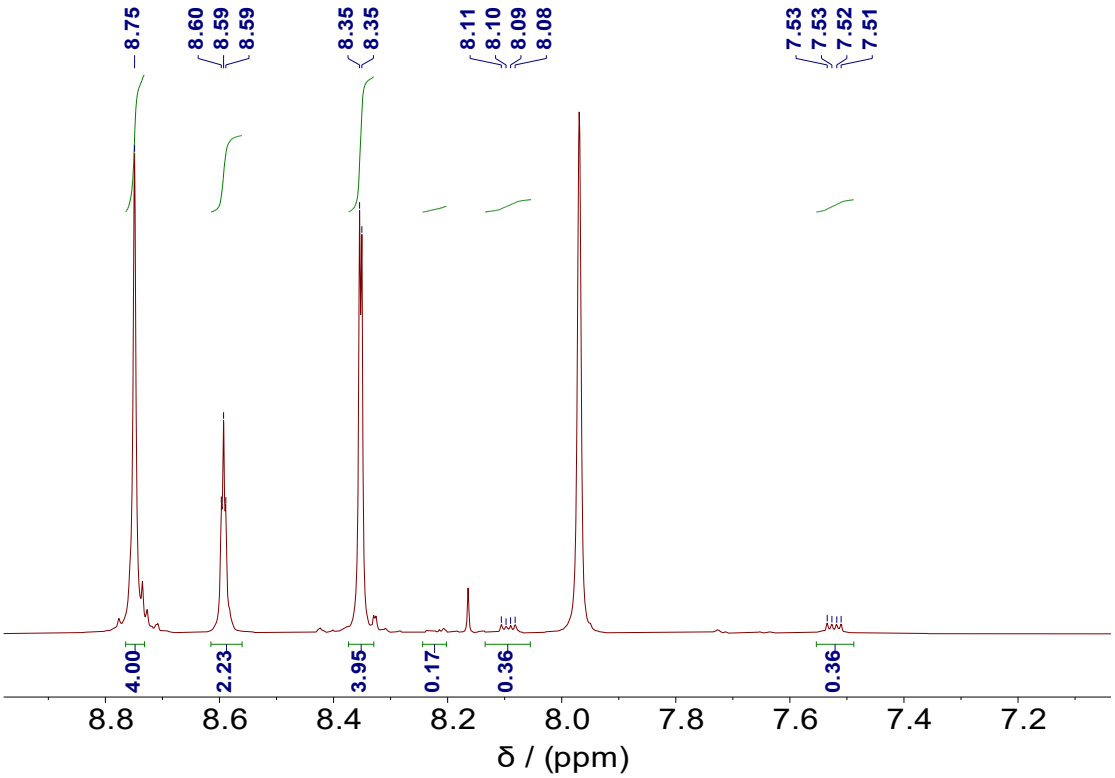


Figure S13. Partial ^{1}H NMR spectrum of Sr-NDI@An in D_2SO_4/DMSO-d_6 after 2 hours of illumination at 635 nm under N_2 atmosphere.

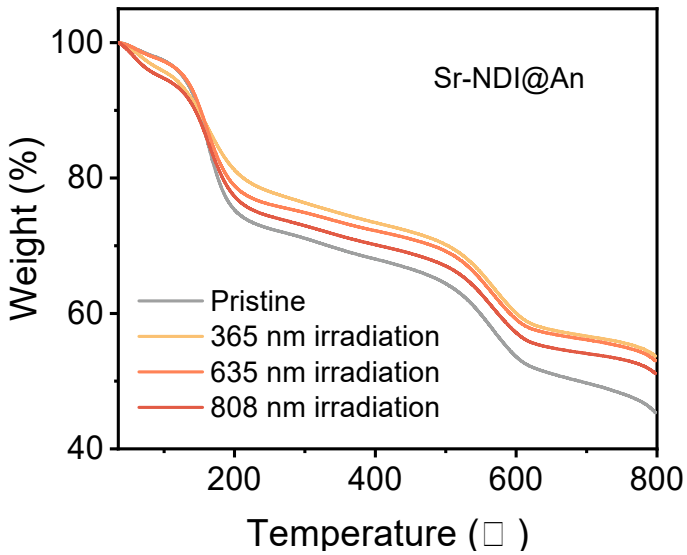


Figure S14. The TGA of Sr-NDI@An and Sr-NDI@An after 365 nm, 635 nm, and 808 nm irradiation.

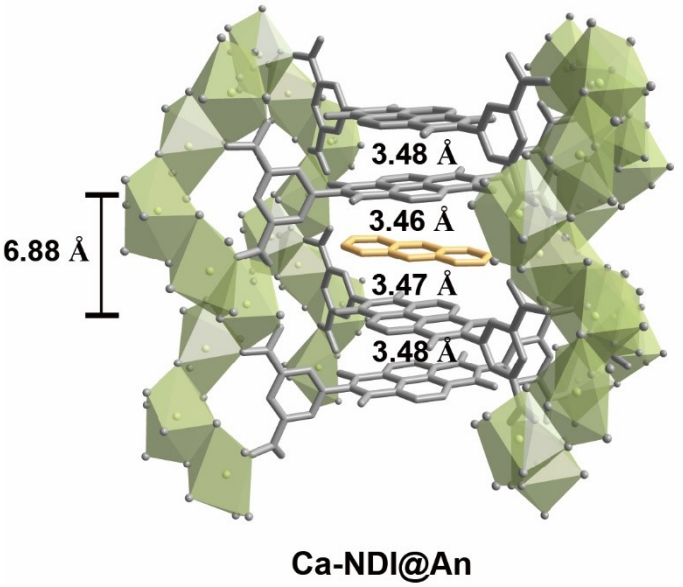


Figure S15. Crystal structures of the MOF cocrystal Ca-NDI@An.

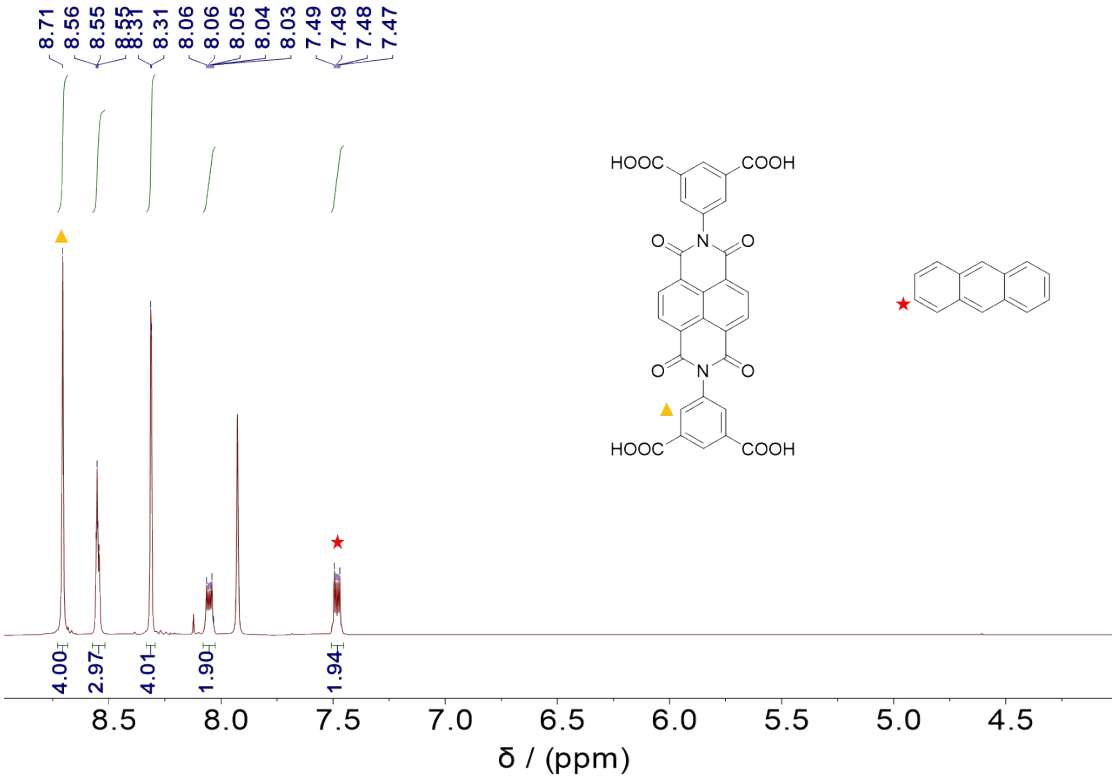


Figure S16. Partial ^{1}H NMR spectrum of Ca-NDI@An in D_2SO_4/DMSO-d_6 after 3 hours of illumination at 365 nm.

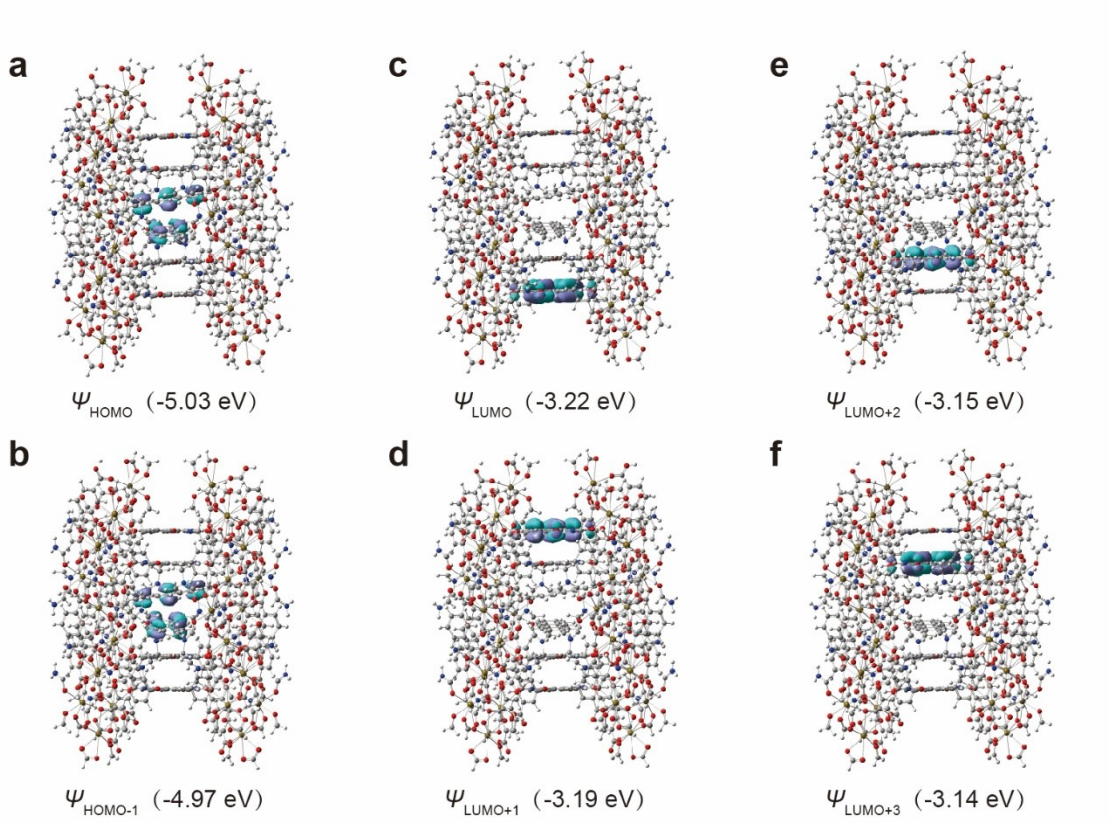


Figure S17. The DFT-calculated molecular orbitals of Sr-NDI@An.

Atomic coordinate data in DFT calculations

O	19.95480	28.10435	-17.96659
O	19.05978	26.36035	-16.92280
C	19.39402	26.97286	-17.96247
N	20.98994	23.53659	-14.91203
C	20.25380	24.45179	-14.26601
H	19.45669	24.97179	-14.86126
Sr	19.58730	28.27176	-15.29965
O	23.76909	26.73098	-20.56440
C	23.02925	26.83814	-17.03253
H	22.25916	27.62923	-17.00774
C	23.41153	26.18840	-15.85981
C	23.65028	26.48683	-18.24228
C	23.32427	27.21445	-19.52747
C	24.96624	24.84686	-17.10111
O	17.80834	26.88759	-14.02735
C	24.40063	25.20214	-15.89547
H	24.70502	24.72490	-14.95589
C	24.58822	25.48637	-18.27246
H	25.05382	25.19640	-19.22169
O	21.63485	27.06040	-14.53759
O	22.66971	28.27460	-19.47261

C	22.76634	26.49963	-14.53347
Sr	21.46744	26.69290	-11.87065
O	19.62538	25.97012	-10.27740
C	19.73253	26.70995	-6.74553
H	20.51785	27.48368	-6.72759
C	19.08280	26.32767	-5.57281
C	19.38124	26.08892	-7.95528
C	20.10885	26.41493	-9.24047
C	17.74126	24.77296	-6.81411
O	22.85161	24.91394	-10.59835
C	18.09654	25.33857	-5.60847
H	17.61701	25.03614	-4.67185
N	22.22632	23.79523	-8.69183
C	18.38077	25.15098	-7.98546
H	18.10031	24.69382	-8.94276
O	19.95480	28.10435	-4.25059
O	21.16900	27.06949	-9.18561
O	19.05978	26.36035	-3.20680
C	19.39402	26.97286	-4.24647
C	22.94256	24.69907	-9.38037
H	23.71676	25.26715	-8.79430
O	20.37602	24.71100	-13.05900
N	20.98994	23.53659	-1.19604
C	20.25380	24.45179	-0.55001
H	19.45359	24.96941	-1.14360
Sr	19.58730	28.27176	-1.58365
O	23.76909	26.73098	-6.84840
C	23.02925	26.83814	-3.31653
H	22.25761	27.62451	-3.29932
C	23.41153	26.18840	-2.14381
C	23.65028	26.48683	-4.52628
C	23.32427	27.21445	-5.81147
C	24.96624	24.84686	-3.38511
O	17.80834	26.88759	-0.31135
C	24.40063	25.20214	-2.17947
H	24.70571	24.72528	-1.24224
N	16.68963	27.51288	-12.12083
C	24.58822	25.48637	-4.55645
H	24.97229	25.23727	-5.36564
C	26.77390	28.34850	-5.90748
H	27.85472	28.62741	-5.81634
H	26.61211	27.32835	-5.46767
O	21.63485	27.06040	-0.82159
O	22.66971	28.27460	-5.75661

O	23.37884	26.16538	-13.49380
C	22.76634	26.49963	-0.81747
C	17.59347	26.79664	-12.80937
H	18.16009	26.02316	-12.22264
O	25.02820	27.48162	-9.63000
N	26.20261	28.09554	-11.48303
C	25.28741	27.35940	-10.83701
H	24.74197	26.58058	-11.42775
C	26.44420	27.89943	-12.88755
H	27.44709	27.42657	-13.05609
H	25.64679	27.24964	-13.35342
Sr	21.46744	26.69290	1.84535
O	19.62538	25.97012	3.43860
C	20.10885	26.41493	4.47553
O	22.85161	24.91394	3.11765
O	21.16900	27.06949	4.53040
C	22.94256	24.69907	4.33563
H	22.42281	25.31798	5.09023
O	20.37602	24.71100	0.65700
O	23.76909	26.73098	6.86760
C	23.32427	27.21445	7.90453
N	16.68963	27.51288	1.59517
O	22.66971	28.27460	7.95939
O	23.37884	26.16538	0.22220
C	17.59347	26.79664	0.90663
H	18.16296	26.02666	1.49510
O	25.02820	27.48162	4.08600
C	25.28741	27.35940	2.87899
H	24.61783	27.73218	2.08206
Sr	21.16616	30.15190	-18.72865
Sr	21.46744	40.90410	-15.56135
O	23.00822	30.87468	-17.13540
O	18.86452	44.32502	-13.72560
O	19.62538	40.18131	-17.15460
C	22.90106	44.34605	-13.82847
H	22.11785	43.56773	-13.84015
C	23.55080	44.72833	-15.00119
C	27.92217	35.02777	-13.77498
C	23.25237	30.75588	-14.81328
C	22.52475	30.42987	-16.09847
C	19.30933	43.84155	-14.76253
C	20.10885	40.62613	-18.19153
O	27.50720	31.44200	-13.77909
C	28.30303	33.68054	-13.78047

C	24.89234	46.28304	-13.75989
O	19.78199	31.93086	-17.45635
O	22.85161	39.12514	-16.83365
C	26.55221	35.43136	-13.78870
O	24.32588	34.68329	-13.78870
C	24.53706	45.71743	-14.96553
H	25.02944	46.02420	-15.89269
C	27.24856	32.63176	-13.75029
C	25.50342	34.39679	-13.76126
C	27.21729	37.74779	-13.80515
H	26.94744	38.81793	-13.81598
C	24.25283	31.69382	-14.84346
H	24.53131	32.15143	-15.80510
C	26.23672	36.77290	-13.82710
H	25.16989	37.06275	-13.87132
O	20.99875	29.78440	-21.39559
O	22.67880	42.95165	-16.32341
O	21.46460	29.77531	-16.04360
O	19.96389	42.78140	-14.81739
O	21.16900	41.28069	-18.24640
O	19.25475	30.67942	-20.35180
O	23.57382	44.69564	-17.36720
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C	23.23957	44.08314	-16.32753
C	19.69104	32.14573	-16.23837
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C	22.94256	38.91027	-18.05163
H	20.21510	31.52984	-15.48304
H	18.21509	41.52390	-15.37760
H	22.46269	39.57709	-18.79017
O	22.25758	32.13380	-19.91700
O	17.60540	29.36318	-16.48800
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C	22.37980	32.39301	-21.12401
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H	22.06137	31.67772	-21.90264
H	18.02726	29.13445	-18.49128
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Sr	19.58730	42.48296	-12.13235
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Sr	23.04630	42.78424	-5.27435

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O	18.86452	30.11382	-13.70640
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O	23.76909	40.94218	-6.86760
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C	19.60435	30.00667	-10.17453
C	22.90106	44.34605	-0.11247
C	19.60435	44.21787	-3.54147
C	19.73253	40.92115	-6.97047
C	23.02925	41.04933	-10.39947
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H	20.37869	29.22341	-10.15566
H	22.11804	43.57128	-0.13110
H	20.37702	43.43160	-3.55885
H	20.51931	41.69235	-6.98727
H	22.25669	41.83517	-10.41558
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O	24.82526	29.95721	-7.16935
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O	22.85161	39.12514	-3.11765
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C	17.34619	29.48540	-3.97901
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C	25.28741	41.57060	-2.87899
H	23.15823	31.84515	-7.99889
H	17.86457	30.28687	-4.57153
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O	23.76909	40.94218	6.84840
C	22.90106	30.13485	0.11247
C	19.60435	30.00667	3.54147
C	19.73253	40.92115	6.74553
C	23.02925	41.04933	3.31653
H	22.11515	29.36245	0.12863
H	20.38269	29.22342	3.55315
H	20.52426	41.69065	6.72050
H	22.25694	41.83514	3.29581
C	23.55080	30.51713	1.28519
C	19.22207	30.65640	4.71419
C	19.08280	40.53887	5.57281

C	23.41153	40.39960	2.14381
N	25.91867	33.07799	0.02057
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C	27.92217	36.02823	3.48798
C	18.98332	30.35797	2.33172
C	23.25237	44.96708	1.09728
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C	19.30933	29.63035	1.04653
C	22.52475	44.64107	2.38247
C	20.10885	40.62613	9.24047
C	23.32427	41.42565	5.81147
O	24.33640	36.44320	3.49209
C	26.57494	35.64737	3.49347
C	24.89234	32.07184	0.04389
C	17.66736	31.99794	3.47289
C	17.74126	38.98416	6.81411
C	24.96624	39.05806	3.38511
O	24.82526	29.95721	6.54665
O	19.78199	46.14206	3.74035
O	17.80834	41.09879	0.31135
O	24.82526	44.16841	7.16935
C	28.32576	37.39819	3.50169
O	27.57769	39.62452	3.50169
C	24.53706	31.50623	1.24953
C	18.23297	31.64266	4.67853
C	18.09654	39.54977	5.60847
C	24.40063	39.41334	2.17947
H	25.01451	31.80335	2.18865
H	17.92622	32.13529	5.60557
H	17.62015	39.24482	4.66864
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C	24.25283	45.90502	1.12746
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C	24.58822	39.69757	4.55645
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H	26.88758	32.27557	3.58472
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O	20.99875	29.78440	6.03641
O	22.67880	42.95165	11.10859
O	20.99875	43.99560	7.67959
O	19.95480	42.31555	4.25059
O	21.63485	41.27160	0.82159
O	19.96389	28.57020	1.10139
O	21.46460	43.98651	2.32761
O	21.16900	41.28069	9.18561
O	22.66971	42.48580	5.75661
O	23.57382	30.48445	3.65120
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O	23.57382	44.69564	10.06480
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O	19.05978	40.57155	3.20680
C	23.23957	29.87194	2.61153
C	19.86726	30.34518	6.04053
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C	19.86726	44.55638	7.67547
C	19.39402	41.18406	4.24647
C	22.76634	40.71083	0.81747
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H	20.24397	36.54310	2.76747
H	21.78993	37.44672	3.13097
H	20.21398	38.34874	3.08065
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C	33.94373	26.70995	-13.82847
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C	33.29400	26.32767	-15.00119
C	37.53547	27.21445	-14.76253
C	31.95246	24.77296	-13.75989
C	32.30774	25.33857	-14.96553
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O	34.16600	28.10435	-16.32341
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Sr	35.67864	26.69290	-8.70335
O	33.83658	25.97012	-10.29660
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H	34.72633	27.48477	-0.13129
H	36.46560	27.62278	-3.55951
C	33.29400	26.32767	-1.28519
C	37.62273	26.18840	-4.71419
C	33.59244	26.08892	-12.61872
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C	34.32005	26.41493	-11.33353
C	37.53547	27.21445	-1.04653
C	31.95246	24.77296	-0.04389
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H	38.91365	24.72306	-5.61583
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H	39.18349	25.23727	-1.49236
H	30.06024	28.33443	-6.86165
C	30.73598	27.45604	-9.93176
H	30.71629	28.50026	-10.34257
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H	29.78862	26.92002	-10.18032
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O	36.88091	28.27460	-1.10139
O	33.27098	26.36035	-3.65120
O	37.59005	26.16538	-7.08020
C	33.60522	26.97286	-2.61153
C	36.97754	26.49963	-6.04053
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H	28.80037	28.06330	-3.01114
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C	33.59244	26.08892	1.09728
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O	37.59005	26.16538	6.63580
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C	32.25658	31.35843	-9.15954
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C	36.97754	40.71083	6.04053
C	39.25133	44.25936	0.90663
C	33.90224	46.35693	4.33563

C	31.80467	41.00784	7.76463
H	38.68015	45.02778	1.49585
H	34.41762	45.73501	5.09106
H	32.47675	41.48262	8.50275
O	31.81660	29.36318	9.63000
O	36.46878	46.34500	0.65700
O	31.81660	43.57438	4.08600
N	35.85486	33.30821	1.19604
C	36.59100	32.39301	0.55001
C	31.55739	29.48540	10.83701
C	31.55739	43.69660	2.87899
H	37.37333	31.85309	1.14016
H	32.27779	29.17442	11.61497
H	32.22677	43.32449	2.08179
C	34.84018	34.08698	0.54590
H	33.96117	34.27247	1.22048
H	35.24682	35.08037	0.21945
C	35.96779	33.44843	2.67476
H	36.37053	34.46105	2.91844
H	34.94982	33.32784	3.13672
H	36.64161	32.65068	3.09043
H	31.11781	46.99217	-17.13642
H	39.88793	47.04069	-6.84940
H	39.93170	38.27051	-10.27912
H	39.92767	38.26442	3.43350
H	31.16216	24.01835	-13.72445
H	31.16518	24.01844	-0.00795
H	39.93456	24.06116	-3.43810
H	37.71092	26.68888	-15.71790
H	39.88507	32.83434	6.84613
H	25.68202	47.03734	-13.72386
H	16.91011	46.99376	-3.43763
H	25.67955	47.03771	-0.00788
H	16.95889	38.22420	-6.86686
H	16.95856	38.22314	6.84933
H	19.21426	26.50389	-18.93995
H	19.37661	30.53099	-22.35706
H	19.58321	26.23934	5.43082
H	16.91303	32.78754	3.43692
H	23.50742	26.66785	8.84681
H	16.95684	24.01542	-6.84937
H	37.28234	30.61299	-19.13395
H	33.41894	26.48053	12.06910
H	38.11938	31.22605	10.38481

H	23.42575	44.57374	12.07006
H	38.53424	40.10563	7.06078
H	33.33672	44.38950	8.84591
H	37.26085	44.81742	5.43128
H	37.44599	26.31888	8.65319
H	19.72747	30.44045	7.95006
H	19.39803	44.73624	8.65283
H	20.11241	40.41317	11.14029
H	37.46810	40.52487	-22.35709
H	37.63055	44.55211	-18.93999
H	33.30617	43.83805	-21.42742
H	19.56241	40.44306	-19.13388
H	19.13366	44.36690	-15.71798
H	23.33700	44.21938	-18.23607
H	23.54302	27.22228	-21.42650
H	33.50660	26.83345	-18.23758
H	34.01356	37.69889	-21.40014
H	40.44139	41.07099	-17.96582
H	40.07560	30.69997	-14.95021
H	33.31612	33.01688	-18.37932
H	22.83205	33.35676	-21.40025
H	16.40345	29.98521	-17.96569
H	23.52784	38.03861	-18.37939
H	16.76036	40.36693	-14.94919
H	26.25125	41.11839	11.11313
H	22.87933	47.54709	7.67884
H	33.26100	47.18995	4.66201
H	30.93043	40.42632	8.09174
H	23.58713	23.86887	4.66253
H	25.91227	30.63288	8.09240
H	30.59081	29.93153	11.11277
H	33.96737	23.50779	7.67837
H	37.81262	38.09125	-15.91109
H	37.10509	33.32837	-12.89578
H	19.04812	32.97780	-15.91218
H	19.74002	37.72755	-12.89583
H	30.98746	26.13567	5.62395
H	25.87083	44.90402	5.62509
H	26.22240	26.84483	2.60872
H	30.62197	44.21054	2.60888
H	16.60443	27.42108	2.60721
H	16.17850	28.27474	1.13949
H	15.97508	27.96321	-4.15256
H	16.29447	28.84158	-5.63272

H	16.63790	27.44510	-11.10247
H	16.19272	28.28753	-12.57071
H	21.76132	23.06323	-14.43219
H	20.87681	23.37092	-15.91186
H	20.89605	23.39764	-2.20351
H	21.77294	23.07619	-0.72275
H	21.44936	23.30155	-9.14083
H	22.29555	23.74351	-7.67386
H	36.50632	23.74311	0.81553
H	35.66228	23.29883	2.28329
H	40.58481	27.97749	5.62307
H	40.89038	28.86404	4.14404
H	35.10353	23.39200	-4.65450
H	35.97086	23.05597	-6.13709
H	35.67594	23.28359	-11.42639
H	36.53098	23.70792	-12.89374
H	40.55726	27.99940	-8.08284
H	40.89625	28.86425	-9.56619
H	40.64655	28.55304	-1.14625
H	40.20373	29.39820	-2.61352
H	40.66960	42.78418	1.13864
H	40.24569	43.64014	2.60584
H	40.54915	42.21481	-5.63307
H	40.86886	43.09361	-4.15309
H	40.65126	42.76769	-12.57035
H	40.20582	43.61026	-11.10234
H	35.07075	47.97842	-0.72304
H	35.94756	47.65695	-2.20389
H	34.55140	47.31088	-7.67369
H	35.39557	47.75402	-9.14141
H	35.08278	47.99191	-14.43244
H	35.96742	47.68442	-15.91207
H	20.31516	47.34642	-12.89412
H	21.16898	47.77217	-11.42634
H	20.85724	47.97489	-6.13417
H	21.73617	47.65568	-4.65416
H	21.18290	47.75663	2.28347
H	20.34139	47.31004	0.81517
H	16.26908	43.07088	5.62597
H	15.96202	42.18530	4.14702
H	16.29178	43.05475	-8.08367
H	15.97095	42.17722	-9.56410
H	39.88595	32.83172	-6.86685
H	25.72653	24.06339	-17.13638

H	31.11868	46.99157	-3.42014
H	16.91219	32.78465	-10.27900
H	25.72567	24.06312	-3.41971
C	30.60808	34.28310	-13.82710
H	31.67481	33.99320	-13.87137

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