Supplementary Information for

The Degradation Mechanism of Multi-Resonance Thermally Activated Delayed Fluorescence Materials

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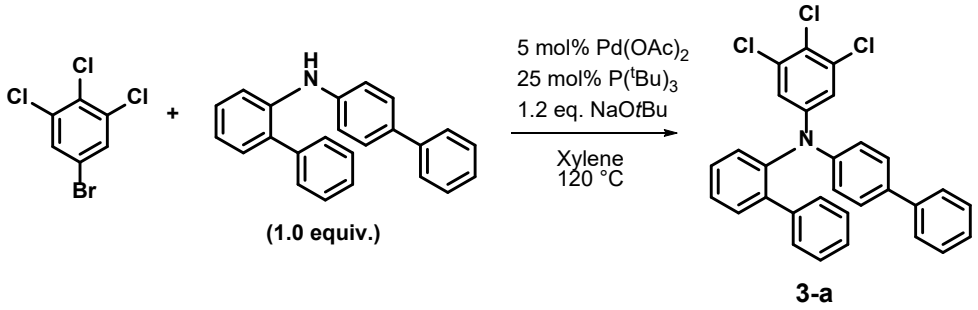
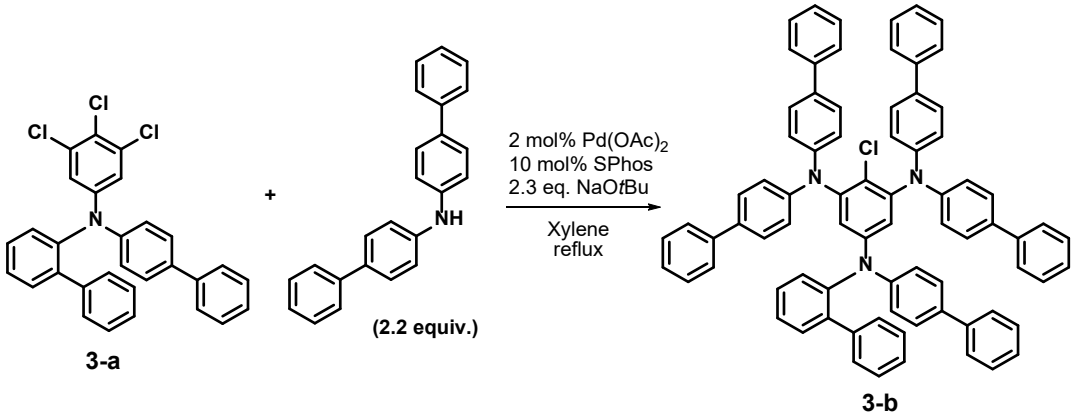
CONTENTS

Supplementary Method 1. Synthesis of **3**.

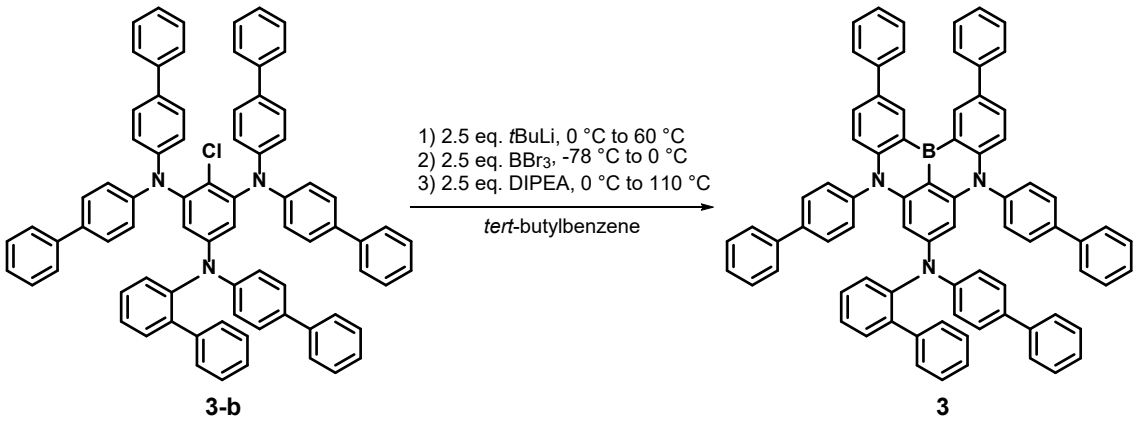


To a stirred solution of 5-bromo-1,2,3-trichlorobenzene (3.90 g, 15.0 mmol), *N*-([1,1'-biphenyl]-4-yl)-[1,1'-biphenyl]-2-amine (4.82 g, 15.0 mmol), palladium(ll) acetate (0.169 g, 0.753 mmol), and sodium *tert*-butoxide (1.73 g, 18.0 mmol) in xylene (30 mL) was added tri-*tert*-butylphosphine (50 wt% in toluene, 1.87 mL, 3.75 mmol) at room temperature under a nitrogen atmosphere. Then the solution was heated to 120 ℃ and stirred for 3 hours. The resulting mixture was cooled down to room temperature. The mixture was diluted with ethyl acetate and a saturated aq. NH_4Cl solution was added. The crude product was then extracted with ethyl acetate, and the collected organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude mixture was purified by column chromatography on silica gel to afford compound **3-a** as white solid (5.89 g, 78%).



The solution of compound **3-a** (5.69 g, 11.3 mmol), di([1,1'-biphenyl]-4-yl)amine (8.00 g, 24.9 mmol), palladium(ll) acetate (0.0507 g, 0.226 mmol), SPhos (0.463 g, 1.13 mmol) and sodium *tert*-butoxide (2.50 g, 26.0 mmol) in xylene (70 mL) was refluxed for 2 hours under a nitrogen atmosphere. The resulting mixture was cooled down to room temperature. The mixture was diluted with ethyl acetate and a saturated aq. NH_4Cl solution was added. The crude product was then extracted with ethyl acetate, and the collected organic layer was dried over $MgSO_4$, filtered, and

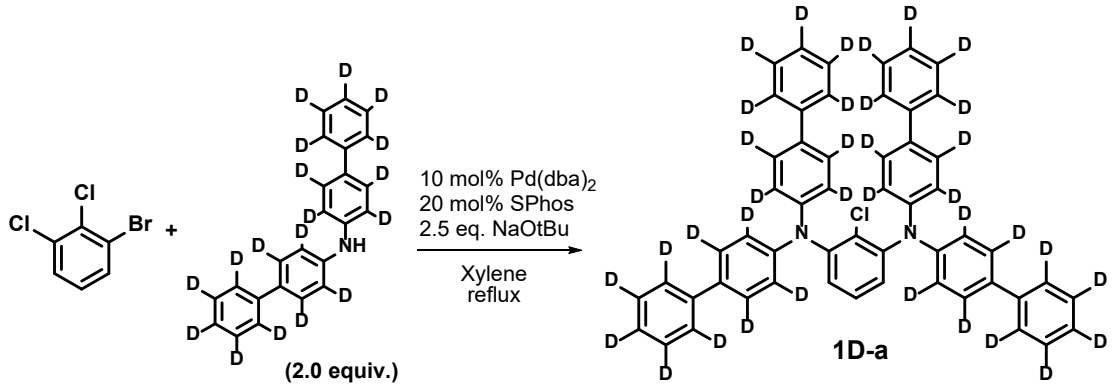
concentrated *in vacuo*. The crude mixture was purified by column chromatography on silica gel to afford compound **3-b** as white solid (10.2 g, 84%).



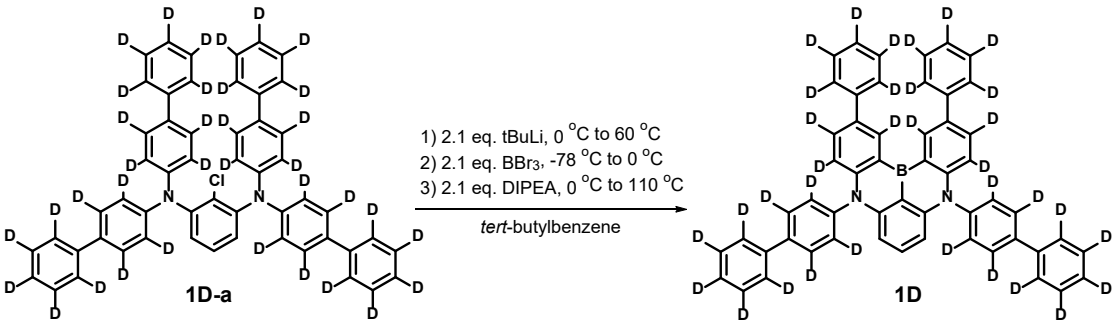
3-b **3**

To a stirred solution of **3-b** (6.19 g, 5.78 mmol) in *tert*-butylbenzene (100 mL) was added *tert*-butyllithium solution (1.7 M in pentane, 8.50 mL, 14.5 mmol) dropwise at 0 ℃ under a nitrogen atmosphere. The resulting mixture was heated to 60 ℃ and stirred for 2 hours. The solution was cooled down to −78 ℃, and boron tribromide (1.40 mL, 14.5 mmol) was added to the solution slowly. The resulting mixture was stirred for an hour at 0 ℃. Diisopropylethylamine (2.50 mL, 14.3 mmol) was added to the reaction mixture at 0 ℃, and, then, the reaction mixture was heated to 110 ℃ and stirred for 3 hours. The solution was cooled down to 0 ℃ and quenched with saturated aq. $NaHCO_3$ solution carefully. The crude product was then extracted with dichloromethane, and the collected organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude mixture was purified by column chromatography on silica gel. Then the obtained product was suspended to ethyl acetate. The suspension was heated to 80 ℃ and stirred for an hour. The insoluble solid was collected by filtration to give **3** as yellow solid (1.8 g, 30%).

Supplementary Method 2. Synthesis of **1D**.



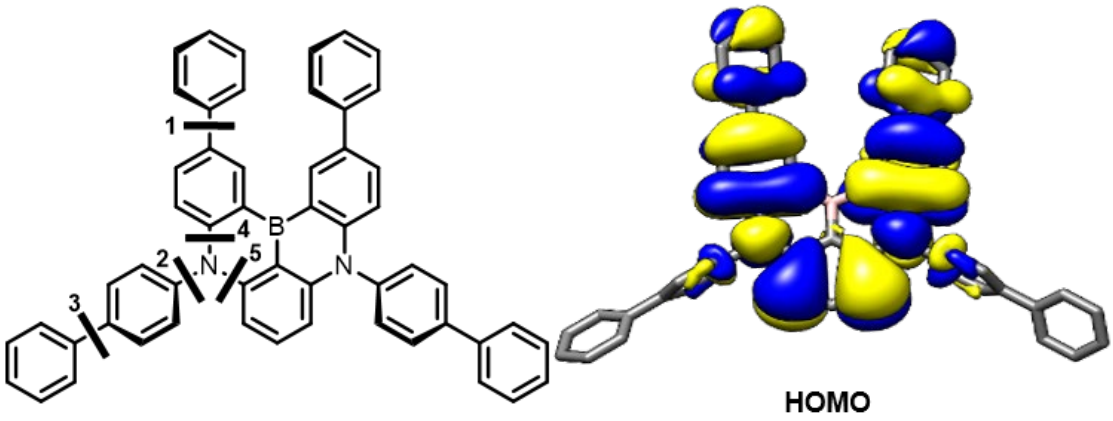
The solution of 1-bromo-2,3-dichlorobenzene (3.30 g, 14.6 mmol), bis(dibenzylidenacetone)palladium(0) (0.840 g, 1.46 mmol), bis([1,1'-biphenyl]-4-yl-d_9)amine (9.91 g, 29.2 mmol), SPhos (1.20 g, 2.92 mmol), and sodium *tert*-butoxide (3.51 g, 36.5 mmol) in xylene (150 mL) was refluxed for 2 hours under a nitrogen atmosphere. The resulting mixture was cooled down to room temperature. The mixture was diluted with ethyl acetate and a saturated aq. NH_4Cl solution was added. The crude product was then extracted with ethyl acetate, and the collected organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude mixture was purified by column chromatography on silica gel to afford compound **1D-a** as white solid (6.2 g, 54%).



To a stirred solution of **1D-a** (3.50 g, 4.45 mmol) in *tert*-butylbenzene (90 mL) was added *tert*-butyllithium solution (1.7 M in pentane, 5.50 mL, 9.35 mmol) dropwise at 0 ℃ under a nitrogen atmosphere. The resulting mixture was heated to 60 ℃ and stirred for an hour. The solution was cooled down to −78 ℃ and boron tribromide (0.90 mL, 9.34 mmol) was added to the solution slowly. The resulting mixture was stirred for 2 hours at 0 ℃. Diisopropylethylamine (1.60 mL, 9.15 mmol) was added to the reaction mixture at 0 ℃, and, then, the reaction mixture was heated to 110 ℃ and stirred for 3 hours. The solution was cooled down to 0 ℃ and quenched with

saturated aq. $NaHCO_3$ solution carefully. The crude product was then extracted with dichloromethane, and the collected organic layer was dried over $MgSO_4$, filtered, and concentrated *in vacuo*. The crude mixture was purified by column chromatography on silica gel. Then the obtained product was recrystallized from dichloromethane/hexane/methanol to give **1D** as yellow solid (0.800 g, 24%).

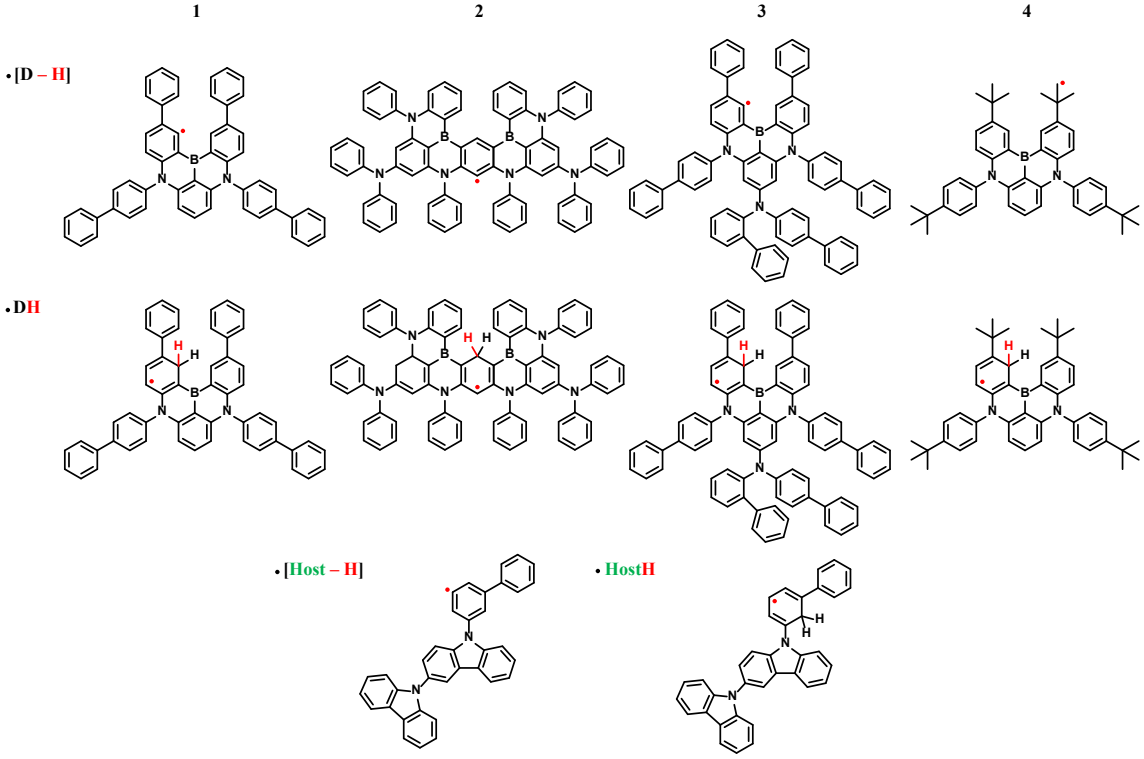
Supplementary Table 1. Calculated bond dissociation free energies (BDFEs) of the neutral (1) and radical cationic species of 1 ($1^{\bullet+}$)



bond	**1** (kcal mol^{-1})	$\mathbf{1}^{\bullet+}$ (kcal mol^{-1})
1	99.67	126.55
2	61.99	65.24
3	101.09	121.30
4	86.43	108.09
5	76.39	89.06

[a]The HOMO of the neutral dopant molecule **1** is depicted with the isodensity value of 0.01 a.u.

Supplementary Table 2. Free energy change for reactions of MR-TADF dopants 1–4[a]



reactions	1	2	3	4
Reaction with a neutral dopant				
$D^{\bullet+} + D \rightarrow [D - H]^+ + \bullet DH$	30.99	30.63	28.05	28.79
$D^{\bullet+} + D \rightarrow [DH]^+ + \bullet[D - H]$	41.70	36.56	33.25	29.65
Reaction with a neutral host molecule				
$D^{\bullet+} + Host \rightarrow [D - H]^+ + \bullet HostH$	33.95	34.54	31.26	31.58
$D^{\bullet+} + Host \rightarrow [DH]^+ + \bullet[Host - H]$	47.36	45.79	40.67	44.49
$D^{\bullet+} + Host \rightarrow \bullet[D - H] + [HostH]^+$ [b]	59.81	65.93	63.32	52.90

[a]Energies in kcal mol^{-1}, calculated at B3LYP-D3/Def2-TZVP//B3LYP-D3/Def2-SVP level of theory. [b]Proton transfer to host molecule.

Supplementary Table 3. Electroluminescence performances of aged devices

1) After LT_{80} operation at an initial luminance of 1000 cd m^{-2}

	V (V)[a]	J (mA cm^{-2})[a]	CIE (x, y)[a]	EQE (%)	power efficiency (lm W^{-1})	luminous efficiency (cd A^{-1})
1	5.48	9.35	(0.12, 0.17)	15.2[b] / 9.20[a]	16.1[b] / 6.17[a]	16.4[b] / 10.7[a]
2	5.62	7.24	(0.11, 0.15)	18.2[b] / 13.7[a]	16.0[b] / 7.73[a]	18.4[b] / 13.8[a]
3	5.56	8.51	(0.13, 0.11)	18.6[b] / 12.8[a]	15.8[b] / 6.66[a]	17.1[b] / 11.8[a]
4	6.52	25.98	(0.13, 0.10)	13.7[b] / 4.40[a]	11.3[b] / 1.86[a]	12.6[b] / 3.85[a]

[a]Values at a luminance of 1000 cd m^{-2}. [b]Maximum values.

2) After LT_{50} operation at an initial luminance of 1000 cd m^{-2}

	V (V)[a]	J (mA cm^{-2})[a]	CIE (x, y)[a]	EQE (%)	power efficiency (lm W^{-1})	luminous efficiency (cd A^{-1})
1	6.25	16.5	(0.12, 0.17)	7.3[b] / 5.2	5.96[b] / 3.05[a]	7.02[b] / 6.07[a]
2	6.22	11.5	(0.12, 0.15)	10.5[b] / 8.6	8.63[b] / 4.40[a]	10.7[b] / 8.71[a]
3	6.32	14.4	(0.13, 0.11)	9.6[b] / 7.5	6.82[b] / 3.45[a]	8.25[b] / 6.94[a]
4	7.51	45.7	(0.14, 0.10)	5.1[b] / 2.5	3.64[b] / 0.91[a]	4.75[b] / 2.19[a]

[a]Values at a luminance of 1000 cd m^{-2}. [b]Maximum values.

Supplementary Table 4. Electroluminescence performances of the 1D device

	V (V)[a]	J (mA cm^{-2})[a]	CIE (x, y)[a]	EQE (%)	power efficiency (lm W^{-1})	luminous efficiency (cd A^{-1})	LT_{95} (h)[c]
1D	5.00	6.81	(0.11, 0.18)	24.0[b] / 12.6[a]	29.9[b] / 9.46[a]	28.6[b] / 15.1[a]	4.41

[a]Values at a luminance of 1000 cd m^{-2}. [b]Maximum values. [c]Operation time when the luminance decreases to 95% of its initial value at initial luminance of 1000 cd m^{-2}.

Supplementary Table 5. DFT-calculated energy components

	***E*(SCF) (eV)**	***ZPE* (kcal mol^{-1})**	***S*(gas) (cal mol^{-1})**
	B3LYP-D3/def2-TZVP	B3LYP-D3/def2-SVP	B3LYP-D3/def2-SVP
1	-60244.966	473.72	236.59
[1–H]'	-60226.497	465.42	238.47
[1+H]'	-60260.066	479.57	240.28
1'+	-60238.999	473.72	238.34
[1–H]+	-60222.572	467.51	232.13
[1+H]+	-60255.609	481.25	237.80
2	-92040.116	700.91	327.02
[2–H]'	-92021.809	692.55	328.16
[2+H]'	-92055.239	706.4	330.91
2'+	-92034.586	701.17	328.36
[2–H]+	-92018.173	695.56	321.11
[2+H]+	-92051.28	708.9	327.25
3	-86894.398	687.38	316.32
[3–H]'	-86875.996	679.16	319.17
[3+H]'	-86909.513	693.22	319.64
3'+	-86888.647	687.2	318.43
[3–H]+	-86872.394	681.76	310.38
[3+H]+	-86905.548	694.96	318.6
4	-52212.979	551.14	244.64
[4–H]'	-52194.867	542.21	247.59
[4+H]'	-52228.086	557.26	248.13
4'+	-52207.121	551.35	246.29
[4–H]+	-52190.8	545.3	240.38
[4+H]+	-52223.858	559.08	246.22
Host	-40694.61894	311.24	173.07
[Host–H]'	-40675.892	302.9	175.78
[Host+H]'	-40709.549	316.71	178.7

Host'+	-40688.229	311.28	174.21
[Host–H]+	-40671.056	304.7	169.18
[Host+H]+	-40704.44041	318.15	175.01
[1–H]+_os	-60220.25224	465.47	237.10
[2–H]+_os	-92015.82812	692.94	327.15
[3–H]+_os	-86869.90899	679.08	316.72
[4–H]+_os	-52188.38537	543.08	245.25
1-TS	-60220.01465	465.12	232.97
2-TS	-92015.51523	692.67	323.06
3-TS	-86869.65393	678.85	315.28
4-TS	-52188.23313	543.03	240.38

Supplementary Table 6. Cartesian coordinates of the DFT-optimized geometries

1

C	-2.591322	-1.334450	-9.198175
C	-1.992052	-0.619506	-8.139196
C	-0.867130	0.195619	-8.457009
C	-0.396949	0.712258	-6.079850
C	-1.499652	-0.079288	-5.647245
C	-2.196860	-1.234945	-10.535483
C	-0.469785	0.332751	-9.810609
C	0.427952	1.355382	-5.135183
C	-1.707799	-0.266425	-4.249684
C	-0.859258	0.355647	-3.314894
C	0.177669	1.165160	-3.777057
H	1.255131	1.988785	-5.449328
H	-1.013734	0.226280	-2.244797
H	0.819837	1.667532	-3.048378
C	-1.129401	-0.355157	-10.818907
H	-3.378246	-2.044487	-8.952111
H	0.364978	0.980189	-10.075541
H	-0.805184	-0.205414	-11.852512
B	-2.441007	-0.711128	-6.657921
N	-0.133087	0.845278	-7.451683
C	1.112921	1.461151	-7.820045
C	1.178386	2.800067	-8.213517
C	2.285140	0.698592	-7.771647
C	2.409302	3.369388	-8.549062
C	3.509555	1.269985	-8.106023
C	3.599971	2.619374	-8.501323
H	0.260908	3.391300	-8.251194
H	2.223160	-0.347492	-7.463600
H	2.446975	4.422707	-8.836030
H	4.408389	0.650555	-8.082396
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C	5.023987	4.185964	-9.876135
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C	6.266392	4.717242	-10.230845
C	7.428489	4.289216	-9.580318
H	6.030219	2.076759	-7.395202
H	4.131088	4.509223	-10.416473
H	8.232326	2.995024	-8.037875
H	6.329785	5.461891	-11.028954
H	8.399506	4.702685	-9.866506
C	-2.872125	-2.038279	-11.587135
C	-2.162598	-2.561760	-12.686300
C	-4.249371	-2.329429	-11.498631
C	-2.797193	-3.354788	-13.646539
C	-4.881734	-3.130222	-12.451368
C	-4.160133	-3.649268	-13.532080
H	-1.090063	-2.370202	-12.775004
H	-4.840488	-1.905867	-10.683580
H	-2.217290	-3.758576	-14.481147
H	-5.949613	-3.344804	-12.349861
H	-4.656013	-4.275065	-14.278671
N	-2.755625	-1.086792	-3.810422
C	-3.714024	-1.362526	-6.060048
C	-3.766891	-1.573859	-4.651688
C	-4.839260	-1.757295	-6.813972
C	-4.866059	-2.274179	-4.095064
H	-4.863456	-1.494557	-7.870772
C	-5.950540	-2.410796	-6.276013
C	-5.924148	-2.683988	-4.891454
H	-4.894860	-2.498176	-3.029873
H	-6.749524	-3.232868	-4.429995
C	-7.098539	-2.790563	-7.134487
C	-6.894748	-3.215721	-8.462813
C	-8.422907	-2.714631	-6.662114
C	-7.972663	-3.525847	-9.293024
C	-9.502106	-3.031001	-7.490561
C	-9.283205	-3.431253	-8.812541
H	-5.877326	-3.324521	-8.846323
H	-8.610577	-2.366667	-5.643039
H	-7.783643	-3.859707	-10.317368
H	-10.521602	-2.950615	-7.102200
H	-10.127644	-3.675411	-9.461799
C	-2.749841	-1.517843	-2.439075
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H	-4.142463	-0.830468	0.591798
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C	-2.849619	-3.026117	1.597792
C	-2.885241	-2.175348	2.718671
C	-2.872202	-4.416736	1.820316
C	-2.934023	-2.695851	4.014291
C	-2.923063	-4.937424	3.115041
C	-2.951769	-4.079356	4.218847
H	-2.849120	-1.092609	2.573236
H	-2.873357	-5.098176	0.965950
H	-2.950584	-2.016377	4.870537
H	-2.948359	-6.020486	3.263649
H	-2.989997	-4.488731	5.231946

[1–H]'

C	-2.724185	-0.943830	-9.169865
C	-2.093940	-0.350662	-8.092424
C	-0.908584	0.382644	-8.417625
C	-0.431524	0.890947	-6.039376
C	-1.572068	0.154381	-5.605674
C	-2.379308	-0.954542	-10.506654
C	-0.518949	0.481591	-9.778808
C	0.404578	1.516494	-5.094859
C	-1.813892	0.002836	-4.209303
C	-0.959462	0.617698	-3.274502
C	0.118842	1.370852	-3.736859
H	1.265914	2.103846	-5.407504
H	-1.138546	0.520997	-2.204557
H	0.768454	1.863686	-3.008276
C	-1.232636	-0.162525	-10.782898
H	0.360763	1.061406	-10.054149
H	-0.890350	-0.048716	-11.816089
B	-2.510831	-0.480835	-6.609808
N	-0.135350	0.976079	-7.411306
C	1.143445	1.520918	-7.780371
C	1.278950	2.852760	-8.181094
C	2.273011	0.696852	-7.734732
C	2.536225	3.354377	-8.525547
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C	3.685635	2.541665	-8.483274
H	0.394150	3.491929	-8.217786
H	2.157407	-0.343868	-7.423939
H	2.627241	4.403343	-8.816257

H	4.387171	0.532447	-8.063927
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C	5.178616	4.044553	-9.857436
C	7.454744	3.041835	-8.591476
C	6.443821	4.512765	-10.220184
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H	6.098439	1.838766	-7.427303
H	4.298849	4.425641	-10.381131
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H	6.538644	5.266487	-11.006555
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C	-3.114318	-1.758576	-11.511183
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C	-4.515936	-3.406615	-13.334359
H	-1.481694	-1.904066	-12.933717
H	-4.930874	-1.836448	-10.336095
H	-2.714457	-3.328149	-14.530844
H	-6.150073	-3.297217	-11.911877
H	-5.053838	-4.047747	-14.037676
N	-2.894441	-0.775864	-3.768819
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C	-3.865886	-1.321097	-4.626404
C	-4.755649	-1.764933	-6.842065
C	-4.976405	-2.014047	-4.085557
H	-4.663556	-1.644219	-7.924298
C	-5.858067	-2.446452	-6.324558
C	-5.944134	-2.555177	-4.918838
H	-5.082231	-2.137597	-3.008578
H	-6.780021	-3.099711	-4.471307
C	-6.888325	-3.044917	-7.208692
C	-6.526968	-3.715040	-8.394080
C	-8.255121	-2.963854	-6.881704
C	-7.498406	-4.292189	-9.215405
C	-9.226659	-3.540845	-7.702405
C	-8.852690	-4.210646	-8.872346
H	-5.471870	-3.803709	-8.664500
H	-8.558971	-2.421392	-5.982428
H	-7.190053	-4.819549	-10.122409
H	-10.282118	-3.460173	-7.426333
H	-9.611153	-4.667620	-9.512925
C	-2.860537	-1.267514	-2.416706
C	-3.566413	-0.645866	-1.382721
C	-2.129486	-2.431069	-2.151250
C	-3.564119	-1.206102	-0.101908
C	-2.122417	-2.981439	-0.872490
C	-2.853654	-2.389939	0.176729
H	-4.142058	0.257254	-1.596483
H	-1.571524	-2.901054	-2.964046
H	-4.156087	-0.735385	0.686384
H	-1.533499	-3.881182	-0.681233
C	-2.888737	-3.021291	1.522344
C	-2.907004	-2.246163	2.697184
C	-2.907238	-4.423690	1.654170
C	-2.936381	-2.850381	3.956581
C	-2.937120	-5.028017	2.912336
C	-2.950180	-4.244343	4.070441
H	-2.872692	-1.156276	2.622489
H	-2.922553	-5.049033	0.758223
H	-2.940153	-2.227864	4.855163
H	-2.958965	-6.118596	2.989064
H	-2.972686	-4.719426	5.054778

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C	-1.061188	0.509520	-8.361787
C	-0.482750	0.822456	-5.982827
C	-1.603879	0.043287	-5.580199
C	-2.615696	-0.390928	-10.646382
C	-0.704198	0.819590	-9.720759
C	0.364165	1.418520	-5.026682
C	-1.816526	-0.167284	-4.186742
C	-0.975751	0.443455	-3.237525
C	0.090921	1.229089	-3.675327
H	1.214655	2.025504	-5.332135
H	-1.144267	0.308501	-2.170682
H	0.735741	1.706774	-2.932676
C	-1.470119	0.379463	-10.801372
H	-4.088400	-0.402193	-9.103323
H	0.187909	1.406697	-9.927041
H	-1.117443	0.650605	-11.798560
B	-2.541323	-0.564585	-6.619103
N	-0.214370	0.981075	-7.347741
C	1.107935	1.417432	-7.714500
C	1.385295	2.750294	-8.031410
C	2.137234	0.470520	-7.760931
C	2.679146	3.127208	-8.399703
C	3.426206	0.850494	-8.127750
C	3.725459	2.186543	-8.459183
H	0.580330	3.487389	-7.990522
H	1.909923	-0.568940	-7.513377
H	2.884218	4.175423	-8.629049
H	4.207932	0.090009	-8.188978
C	5.100623	2.579922	-8.865941
C	6.227646	1.970899	-8.279887
C	5.315931	3.560050	-9.854063
C	7.521159	2.329017	-8.666662
C	6.609206	3.919160	-10.241605
C	7.718283	3.305483	-9.649484
H	6.087650	1.222076	-7.496470
H	4.459802	4.028780	-10.345043
H	8.378308	1.844793	-8.190748
H	6.753607	4.675575	-11.017756
H	8.728635	3.588930	-9.957411
C	-3.389059	-0.920229	-11.773329
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C	-4.449603	-1.838736	-11.568799
C	-3.808691	-1.110607	-14.182584
C	-5.152668	-2.391568	-12.640713
C	-4.835755	-2.038121	-13.955792
H	-2.314593	0.160336	-13.331297
H	-4.734836	-2.144592	-10.561708
H	-3.553134	-0.807636	-15.202210
H	-5.956582	-3.105054	-12.438961
H	-5.386530	-2.474112	-14.793127
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C	-3.760607	-1.640000	-4.631832
C	-4.630973	-2.150501	-6.828928
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C	-5.646082	-3.163679	-4.913125
H	-4.819331	-2.650099	-3.015020
H	-6.370894	-3.843338	-4.457911
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C	-6.073278	-4.260796	-8.451536
C	-7.835966	-4.073390	-6.814817
C	-6.910764	-5.023158	-9.268626

C	-8.671892	-4.843399	-7.626859
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H	-5.047141	-4.067064	-8.773460
H	-8.217627	-3.680471	-5.868902
H	-6.534893	-5.399475	-10.224461
H	-9.689115	-5.069558	-7.294068
H	-8.865445	-5.933552	-9.489335
C	-2.898275	-1.364954	-2.373280
C	-3.700987	-0.664705	-1.468234
C	-2.126843	-2.443703	-1.926047
C	-3.740014	-1.053499	-0.127081
C	-2.166167	-2.827627	-0.586920
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H	-4.305023	0.171195	-1.827770
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H	-4.393064	-0.518724	0.566515
H	-1.544744	-3.659679	-0.247997
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C	-3.073321	-1.623665	2.802052
C	-3.027101	-3.935396	2.104353
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C	-3.099646	-3.388785	4.464205
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H	-3.017775	-4.688556	1.312302
H	-3.126401	-1.276510	4.931791
H	-3.068914	-5.406595	3.684856
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C	-2.072673	-1.581122	-10.615152
C	-0.259931	-0.099446	-9.906439
C	0.596419	1.018628	-5.257709
C	-1.576173	-0.544215	-4.374794
C	-0.699293	0.055380	-3.436783
C	0.354605	0.843350	-3.897399
H	1.425713	1.644469	-5.580507
H	-0.858532	-0.071254	-2.367049
H	1.007098	1.336723	-3.173929
C	-0.931016	-0.787472	-10.898906
H	-3.371970	-2.233894	-9.043215
H	0.627709	0.475645	-10.164825
H	-0.565053	-0.714118	-11.925581
B	-2.360574	-0.931885	-6.770693
N	0.034031	0.482181	-7.565374
C	1.226863	1.211605	-7.945525
C	1.133057	2.537305	-8.376228
C	2.476385	0.594356	-7.830957
C	2.297432	3.251644	-8.662039
C	3.634353	1.318348	-8.110979
C	3.571254	2.665753	-8.520118
H	0.153104	3.010898	-8.469770
H	2.535321	-0.445749	-7.501775
H	2.218434	4.295954	-8.971409
H	4.605054	0.826432	-8.019137
C	4.808783	3.450532	-8.766088
C	5.930307	3.295221	-7.928052
C	4.884633	4.376798	-9.824178
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C	6.047306	5.120479	-10.039737
C	7.152572	4.958241	-9.197677
H	5.885017	2.603115	-7.083129
H	4.034276	4.502790	-10.499334
H	7.946545	3.913705	-7.473372
H	6.094072	5.825486	-10.873611
H	8.061256	5.540670	-9.369836
C	-2.745415	-2.386169	-11.659094
C	-2.009561	-2.997279	-12.696030
C	-4.140976	-2.593140	-11.623998
C	-2.641200	-3.798828	-13.648896
C	-4.771303	-3.392664	-12.577471
C	-4.024707	-4.002806	-13.592660
H	-0.924379	-2.875277	-12.737152
H	-4.742876	-2.096052	-10.859214
H	-2.047348	-4.276263	-14.432156
H	-5.853567	-3.539694	-12.531819
H	-4.520178	-4.631562	-14.336449
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C	-3.669243	-1.481990	-6.156548
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H	-4.884697	-1.426052	-7.917818
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C	-5.924188	-2.662859	-4.931038
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C	-8.515978	-2.451116	-6.385946
C	-8.482512	-2.572835	-9.172335
C	-9.715114	-2.529713	-7.093259
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H	-6.343277	-2.502910	-9.018897
H	-8.551843	-2.376018	-5.297329
H	-8.465530	-2.631505	-10.263648
H	-10.662874	-2.535595	-6.549393
H	-10.643461	-2.647167	-9.047590
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C	-3.436032	-0.981752	-1.598369
C	-1.940519	-2.816797	-2.129279
C	-3.477541	-1.410819	-0.270793
C	-1.982831	-3.233897	-0.799455
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C	-2.852529	-4.401668	1.850916
C	-2.934709	-2.567419	3.953221
C	-2.914700	-4.854339	3.170343
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H	-2.845136	-5.128374	1.034548
H	-2.957751	-1.845991	4.773800
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C	-1.143371	-1.007065	-6.229641

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C	-0.268118	-0.367851	-3.976358
C	0.844895	0.188716	-4.508431
H	1.844040	-0.930584	-5.934111
H	-0.462446	-0.272946	-2.908452
H	1.558167	0.716994	-3.870315
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H	-3.551124	-2.446037	-9.404294
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H	-0.712244	-1.298308	-12.412862
B	-2.279555	-1.363401	-7.170488
N	0.190503	-0.137687	-8.059580
C	1.304144	0.776231	-8.158785
C	1.877393	0.938512	-6.878874
C	1.787286	1.516614	-9.238248
C	2.938759	1.804150	-6.668899
C	2.859174	2.389530	-9.014073
C	3.457198	2.550248	-7.749174
H	1.336446	1.472853	-10.226570
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H	3.222011	2.992732	-9.849036
C	4.600071	3.478481	-7.552325
C	5.650474	3.527694	-8.489477
C	4.665871	4.316641	-6.422081
C	6.736067	4.386512	-8.299733
C	5.748940	5.179707	-6.236914
C	6.788595	5.215418	-7.172992
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H	7.549721	4.399767	-9.029740
H	5.781244	5.829748	-5.358790
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C	-3.094636	-2.651656	-12.042908
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C	-3.276655	-4.107368	-13.993983
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C	-4.610790	-2.558980	-4.361367
H	-4.911399	-1.697749	-8.115746
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C	-5.801344	-2.784312	-5.035190
H	-4.543982	-2.815718	-3.305220
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C	-9.724692	-2.566354	-6.970171
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H	-10.637735	-2.527360	-6.370937
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C	-1.772398	-2.801529	-2.209879
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C	-1.807918	-2.925417	-0.820783
C	-2.513438	-2.002617	-0.022032
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C	-2.560904	-3.407370	2.067602
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C	-0.353829	0.043196	-9.899907
C	0.836871	0.740473	-5.224409
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C	0.510906	0.494753	-3.794219
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H	-3.383661	-2.224062	-9.093896
H	0.504197	0.667134	-10.146653
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C	1.219772	1.181374	-7.893397
C	1.139612	2.568157	-8.041378
C	2.442573	0.523620	-8.054100
C	2.297293	3.300243	-8.309374
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C	3.549562	2.667498	-8.440813
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H	2.231242	4.386871	-8.395088
H	4.541203	0.739299	-8.461856
C	4.784737	3.449042	-8.701329
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C	-2.703513	-3.593724	-13.742195
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H	5.034795	-2.119075	-14.659019
C	3.534404	-4.453139	-11.960314
C	4.867283	-4.066003	-11.875318
H	6.428088	-2.869022	-12.786966
H	3.151721	-5.149294	-11.214799
H	5.498730	-4.438201	-11.065485
C	3.710094	-2.713256	-17.259334
C	3.320633	-0.621962	-16.082434
C	4.371724	-2.017420	-18.274397
H	3.585578	-3.797054	-17.312498
C	4.001596	0.065671	-17.091558
H	2.907124	-0.092596	-15.221290
C	4.522226	-0.628491	-18.189601
H	4.771271	-2.564917	-19.130981
H	4.128148	1.148494	-17.016808
H	5.048053	-0.085414	-18.978481
H	2.391862	-2.185147	-21.929475
H	-6.172276	-1.017256	-19.262327
H	-5.465852	-6.053844	-17.306692
H	1.488727	-5.145361	-10.461525

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C	-5.579386	-9.066169	-12.214963
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H	-1.937774	-9.792028	-11.049008
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C	-3.528809	-3.713279	-18.496759
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H	2.214950	1.405168	-10.226408
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H	-3.840246	-6.484842	-20.465204
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C	-1.059215	-1.520617	-4.207845
C	-0.096587	-1.280264	-3.222559
C	1.127340	-0.694936	-3.573557
H	2.351704	0.093950	-5.148861
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H	-3.291984	-1.655661	-9.030104
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B	-1.952267	-1.255809	-6.587290
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C	1.849815	0.619749	-7.464443
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C	3.096838	-0.010885	-7.528465
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C	5.600245	4.015247	-8.697624
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H	6.394440	1.919341	-6.126463
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H	6.879681	5.574421	-9.474554
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C	-4.305710	-0.975774	-11.437769
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H	-6.265504	-1.077227	-12.326807
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C	-3.382046	-2.202975	-4.691316
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C	-4.580949	-2.773946	-4.203037
H	-4.562222	-1.172780	-7.708274
C	-5.769676	-2.153422	-6.240785
C	-5.736382	-2.755794	-4.964616
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C	-8.243348	-1.992888	-9.137134
C	-9.478510	-1.931305	-7.066181
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H	-3.724587	-1.688066	0.504583
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C	-2.794717	-3.181676	2.656160
C	-3.056355	-5.417911	1.787336
C	-2.987660	-3.662002	3.952934
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C	-3.216816	-5.023232	4.174324
H	-2.581869	-2.121221	2.501852
H	-3.115613	-6.110308	0.944188
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C	2.649340	1.966438	-3.168397
C	5.377124	1.285020	-2.794171
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C	5.027270	2.566681	-3.231706
H	6.424673	1.014501	-2.635148
H	3.413953	3.900706	-3.732710
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C	2.039912	-1.055907	-1.320973
C	1.892089	-2.453071	-1.252237
C	1.995604	-0.984978	1.108380
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C	1.744478	-3.090798	-0.024466
H	1.862017	-3.032066	-2.176828
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C	0.973933	-4.270709	4.974466
H	-0.381987	-5.536603	3.856367
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H	0.745125	-4.737842	5.936457
H	5.797628	3.317451	-3.422002
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C	-1.056081	-1.400298	-4.184455
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H	4.988326	3.773683	-9.744387
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C	-4.643436	-0.303367	-11.099948
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C	-5.620503	-0.337759	-12.095821
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H	-6.675225	-0.296025	-11.809102
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H	-7.416400	-2.712097	-10.699155
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H	-9.772535	-2.846662	-9.848842
C	-2.371695	-2.487923	-2.457357
C	-3.028115	-1.734673	-1.478790
C	-1.801886	-3.718528	-2.114268
C	-3.133445	-2.221553	-0.174854
C	-1.897051	-4.194644	-0.806705
C	-2.574415	-3.462472	0.187515
H	-3.475580	-0.777922	-1.757421
H	-1.273440	-4.289857	-2.880364
H	-3.683327	-1.640787	0.568933
H	-1.426503	-5.146601	-0.549867
C	-2.717911	-3.994137	1.568423
C	-2.662376	-3.141868	2.686948
C	-2.925481	-5.368639	1.793008
C	-2.814791	-3.642804	3.981233
C	-3.077069	-5.870605	3.088040
C	-3.024634	-5.009299	4.188366
H	-2.464463	-2.077267	2.541085
H	-2.999878	-6.048875	0.941144
H	-2.751789	-2.963365	4.834797
H	-3.251532	-6.939677	3.237912
H	-3.143919	-5.404485	5.200747
N	2.065764	-0.234699	-2.573724
C	4.340214	0.567739	-2.423839
C	2.990973	0.840684	-2.710324
C	2.602173	2.150968	-3.098846
C	5.314118	1.559035	-2.507612
H	4.611119	-0.448449	-2.128849
C	3.614122	3.126770	-3.197869
C	4.948270	2.849591	-2.902774
H	6.354186	1.320291	-2.269522
H	3.328096	4.142659	-3.480384
C	2.003965	-0.228500	-0.121150
C	2.033550	-0.931641	-1.335992
C	1.990535	-2.336126	-1.301501
C	1.888516	-0.911961	1.088238
H	2.050550	0.862637	-0.132732
C	1.854410	-3.009692	-0.091487
H	2.036666	-2.892425	-2.239604
C	1.783109	-2.315105	1.131786
H	1.825209	-0.337123	2.015258
H	1.819370	-4.101628	-0.090550
C	1.566843	-3.033723	2.411929
C	0.729000	-4.164765	2.467186
C	2.159847	-2.588642	3.609257
C	0.483596	-4.819871	3.675116
H	0.226008	-4.509119	1.561345
C	1.913026	-3.241662	4.819081
H	2.834940	-1.729554	3.587552
C	1.070078	-4.358362	4.857762
H	-0.195917	-5.674737	3.693215
H	2.387429	-2.875934	5.734273
H	0.863401	-4.864466	5.804780
H	-0.282352	-1.359572	-2.167684
H	5.697352	3.642178	-2.971102
C	1.198047	2.538477	-3.413352
C	0.933151	3.357839	-4.527479
C	0.106700	2.115480	-2.632291
C	-0.371899	3.723854	-4.863268
C	-1.199707	2.472078	-2.972680
C	-1.448137	3.274307	-4.091487
H	1.763245	3.684669	-5.156849
H	0.279169	1.484109	-1.759814
H	-0.552888	4.350447	-5.741121
H	-2.029136	2.109447	-2.359724
H	-2.470767	3.548002	-4.365151

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C	0.483741	-0.614310	-5.996830
C	-0.782936	-1.166157	-5.644432
C	-2.083156	-0.546649	-10.513706
C	0.146909	-0.017174	-9.678946
C	1.481688	-0.431284	-5.028243
C	-0.989958	-1.515836	-4.281916
C	-0.013751	-1.273027	-3.307759
C	1.219385	-0.729748	-3.683653
H	2.444891	-0.006679	-5.289404
C	-0.764598	-0.091839	-10.721124
H	-3.404271	-1.337512	-9.040284
H	1.152264	0.346100	-9.888779
H	-0.442504	0.239368	-11.710770

B	-1.904290	-1.306184	-6.659093
N	0.721894	-0.231922	-7.328579
C	1.943690	0.473237	-7.605195
C	1.928102	1.866388	-7.740792
C	3.161119	-0.210302	-7.686507
C	3.120878	2.569767	-7.907897
C	4.356351	0.498896	-7.818153
C	4.359573	1.902538	-7.916680
H	0.971785	2.390097	-7.693306
H	3.163556	-1.299423	-7.605917
H	3.100429	3.659660	-7.988415
H	5.304008	-0.043676	-7.858468
C	5.635368	2.660988	-8.006562
C	6.697972	2.369454	-7.129563
C	5.807862	3.688699	-8.952740
C	7.900040	3.077558	-7.204711
C	7.013363	4.391497	-9.032616
C	8.063900	4.086798	-8.160346
H	6.565278	1.597948	-6.366653
H	4.994826	3.924344	-9.644874
H	8.711737	2.840303	-6.511159
H	7.137215	5.177646	-9.782425
H	9.007441	4.634847	-8.227867
C	-3.084266	-0.603313	-11.610043
C	-2.695264	-0.678702	-12.962537
C	-4.468176	-0.574983	-11.335181
C	-3.640391	-0.717894	-13.989660
C	-5.414615	-0.623121	-12.359385
C	-5.007137	-0.692142	-13.695684
H	-1.634910	-0.725503	-13.220481
H	-4.817389	-0.485180	-10.304342
H	-3.302583	-0.777510	-15.028300
H	-6.478564	-0.591341	-12.106295
H	-5.746683	-0.723511	-14.499789
N	-2.210284	-2.079092	-3.896445
C	-3.239419	-1.834773	-6.104149
C	-3.304864	-2.219469	-4.762223
C	-4.488715	-1.982738	-6.949563
C	-4.509213	-2.786864	-4.219287
H	-4.682441	-1.025445	-7.470120
C	-5.761700	-2.433337	-6.285493
C	-5.686866	-2.856564	-4.965838
H	-4.520532	-3.166265	-3.200185
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C	-7.011645	-2.431899	-7.050414
C	-7.012079	-2.317514	-8.461864
C	-8.273812	-2.516622	-6.411894
C	-8.203639	-2.304081	-9.188803
C	-9.461283	-2.495834	-7.138609
C	-9.436873	-2.391150	-8.535672
H	-6.070941	-2.253924	-9.009791
H	-8.325665	-2.573349	-5.322754
H	-8.165144	-2.224084	-10.278981
H	-10.416276	-2.552537	-6.608756
H	-10.368553	-2.372015	-9.106654
C	-2.335121	-2.517937	-2.532696
C	-2.974480	-1.715573	-1.581515
C	-1.809471	-3.755143	-2.146332
C	-3.124341	-2.167684	-0.269570
C	-1.946527	-4.195957	-0.829460
C	-2.622920	-3.420880	0.132719
H	-3.381806	-0.750359	-1.890668
H	-1.289049	-4.364907	-2.887994
H	-3.668295	-1.549308	0.447839
H	-1.515323	-5.157675	-0.542003
C	-2.829766	-3.921442	1.518007
C	-2.803479	-3.048849	2.622139
C	-3.075081	-5.286837	1.761469
C	-3.019740	-3.520546	3.918481
C	-3.289049	-5.760053	3.058706
C	-3.265243	-4.878332	4.143827
H	-2.578482	-1.991275	2.465573
H	-3.129620	-5.983277	0.921371
H	-2.979963	-2.824791	4.760260
H	-3.492690	-6.822120	3.221352
H	-3.435585	-5.250756	5.157594
N	2.179835	-0.417105	-2.697670
C	4.502185	0.267538	-2.772804
C	3.147939	0.603072	-2.932976
C	2.785192	1.909668	-3.357601
C	5.510228	1.190187	-3.044733
H	4.749624	-0.743673	-2.441840
C	3.825950	2.808203	-3.661063
C	5.169709	2.464712	-3.509914
H	6.557426	0.905084	-2.910240
H	3.564958	3.813322	-4.000222
C	2.275718	-0.326243	-0.247542
C	2.155292	-1.064335	-1.437503
C	1.960788	-2.454505	-1.342116
C	2.131666	-0.950225	0.990890
H	2.456356	0.749578	-0.298193
C	1.795021	-3.064153	-0.102910
H	1.903993	-3.048285	-2.255904
C	1.849461	-2.325471	1.095378
H	2.184429	-0.339482	1.895187
H	1.628501	-4.142972	-0.061399
C	1.574561	-2.963825	2.406568
C	0.627468	-4.001391	2.513122
C	2.213791	-2.529009	3.584335
C	0.322881	-4.575280	3.748741
H	0.086163	-4.333806	1.625313
C	1.905895	-3.098298	4.822149
H	2.972740	-1.744865	3.525324
C	0.955298	-4.122240	4.910741
H	-0.438228	-5.356832	3.803860
H	2.416978	-2.740575	5.720615
H	0.701910	-4.563914	5.878654
H	-0.221527	-1.466493	-2.261261
H	-4.266144	-2.686278	-7.780035
H	5.946983	3.194307	-3.748213
C	1.370458	2.346635	-3.526362
C	1.000684	3.113237	-4.647808
C	0.368029	2.010011	-2.597511
C	-0.324280	3.503826	-4.851489
C	-0.957514	2.398316	-2.801217
C	-1.313339	3.139251	-3.932817
H	1.758484	3.374597	-5.387603
H	0.621580	1.421432	-1.715360
H	-0.589584	4.084219	-5.739531
H	-1.718220	2.108796	-2.071462
H	-2.352926	3.433413	-4.100465

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C	-2.437557	-1.061277	-9.142094
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C	0.245098	-0.262874	-5.863315
C	-1.002276	-0.860430	-5.530328
C	-2.006869	-0.856786	-10.459332
C	0.030916	0.142508	-9.560956
C	1.245758	-0.075180	-4.882584
C	-1.189880	-1.277747	-4.188595
C	-0.194527	-1.077492	-3.211633

C	1.033128	-0.482771	-3.555868
H	2.184432	0.407418	-5.132706
H	-0.382331	-1.344265	-2.176894
C	-0.757708	-0.214693	-10.639085
H	-3.378167	-1.588753	-8.991732
H	0.996776	0.611860	-9.741632
H	-0.399854	0.002262	-11.648276
B	-2.105723	-1.003707	-6.549031
N	0.479756	0.144557	-7.174629
C	1.699241	0.875856	-7.445014
C	1.649579	2.263783	-7.603186
C	2.928377	0.210321	-7.483152
C	2.834651	2.988250	-7.740411
C	4.109959	0.943909	-7.589306
C	4.087718	2.348323	-7.697046
H	0.683804	2.772153	-7.585786
H	2.953778	-0.877868	-7.392413
H	2.792927	4.075968	-7.834986
H	5.068380	0.420117	-7.598002
C	5.350696	3.130683	-7.739762
C	6.391190	2.843229	-6.834850
C	5.529949	4.174662	-8.666528
C	7.580434	3.575474	-6.862328
C	6.724646	4.898944	-8.699912
C	7.752956	4.600609	-7.799268
H	6.254579	2.056576	-6.088005
H	4.736192	4.406268	-9.382036
H	8.376093	3.343556	-6.149140
H	6.857836	5.696742	-9.435108
H	8.687540	5.166330	-7.830025
C	-2.802770	-1.346250	-11.607090
C	-2.166616	-1.904165	-12.734776
C	-4.212478	-1.310783	-11.585917
C	-2.910620	-2.422842	-13.795919
C	-4.955202	-1.822162	-12.650844
C	-4.309112	-2.386062	-13.757436
H	-1.076035	-1.967452	-12.764690
H	-4.731464	-0.852048	-10.740304
H	-2.394837	-2.867053	-14.651139
H	-6.047001	-1.775382	-12.620347
H	-4.893899	-2.792814	-14.586058
N	-2.383209	-1.880626	-3.807365
C	-3.470415	-1.474239	-5.981336
C	-3.500421	-1.968814	-4.636518
C	-4.691223	-1.450941	-6.682198
C	-4.692315	-2.549013	-4.128635
H	-4.705729	-0.978739	-7.663398
C	-5.896831	-1.952567	-6.168947
C	-5.848528	-2.543479	-4.879819
H	-4.705569	-3.001439	-3.139185
H	-6.739351	-3.017424	-4.464274
C	-7.164701	-1.888001	-6.928980
C	-7.177676	-1.851633	-8.339697
C	-8.406089	-1.865102	-6.257959
C	-8.379379	-1.805987	-9.046094
C	-9.607579	-1.815611	-6.964466
C	-9.600629	-1.789105	-8.363126
H	-6.238889	-1.894256	-8.895817
H	-8.434496	-1.861670	-5.166209
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H	-10.540750	-1.755741	-8.919004
C	-2.470131	-2.411617	-2.463225
C	-3.086345	-1.668458	-1.451814
C	-1.922082	-3.665335	-2.179071
C	-3.168978	-2.192564	-0.161793
C	-2.000208	-4.176878	-0.883395
C	-2.632726	-3.458747	0.150675
H	-3.516575	-0.692315	-1.687533
H	-1.427974	-4.230129	-2.972598
H	-3.683938	-1.619817	0.611937
H	-1.548630	-5.147580	-0.668402
C	-2.750792	-4.024628	1.519284
C	-2.666854	-3.198660	2.655805
C	-2.963407	-5.403238	1.711904
C	-2.796352	-3.730531	3.939881
C	-3.094968	-5.934791	2.996817
C	-3.013295	-5.100247	4.115856
H	-2.465164	-2.131572	2.535048
H	-3.062363	-6.063805	0.847226
H	-2.713592	-3.073520	4.808852
H	-3.276244	-7.005192	3.124743
H	-3.117772	-5.518843	5.120148
N	1.990927	-0.256440	-2.570746
C	4.335453	0.371860	-2.532469
C	2.997182	0.749004	-2.724457
C	2.672937	2.086691	-3.068863
C	5.367065	1.295819	-2.687826
H	4.554705	-0.662480	-2.258242
C	3.737336	2.988316	-3.255665
C	5.066451	2.609129	-3.064085
H	6.402011	0.985513	-2.522002
H	3.504842	4.021017	-3.526008
C	1.981958	-0.351177	-0.115177
C	1.959571	-1.005783	-1.355274
C	1.879925	-2.407595	-1.380033
C	1.870566	-1.081536	1.067288
H	2.076848	0.736249	-0.079561
C	1.753701	-3.128095	-0.194880
H	1.903205	-2.929476	-2.339335
C	1.725415	-2.482900	1.057042
H	1.852866	-0.543820	2.017741
H	1.697397	-4.217904	-0.238218
C	1.526126	-3.250109	2.312218
C	0.690866	-4.384234	2.335222
C	2.138908	-2.851943	3.515962
C	0.469516	-5.089733	3.518836
H	0.173240	-4.696424	1.425995
C	1.916230	-3.555875	4.701372
H	2.814383	-1.993157	3.521362
C	1.077495	-4.676112	4.708252
H	-0.203558	-5.949582	3.513796
H	2.406567	-3.227900	5.621943
H	0.892755	-5.223041	5.636537
H	5.864766	3.342564	-3.197196
C	1.272200	2.550398	-3.274328
C	0.952431	3.327631	-4.403101
C	0.236081	2.217795	-2.381900
C	-0.361942	3.733629	-4.650047
C	-1.077990	2.617853	-2.630513
C	-1.385735	3.371367	-3.770180
H	1.742107	3.590581	-5.108646
H	0.456892	1.625354	-1.492982
H	-0.588683	4.332012	-5.536627
H	-1.866454	2.340817	-1.925729
H	-2.414448	3.684165	-3.967691

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C	-0.973439	-0.923919	-5.649690

C	-2.066058	-0.716328	-10.575716
C	0.043006	0.123872	-9.676119
C	1.286854	0.121339	-5.075905
C	-1.094372	-1.302137	-4.279594
C	-0.014933	-1.124193	-3.368488
C	1.163093	-0.477198	-3.693630
H	0.976055	1.182210	-4.922939
H	-0.144904	-1.459394	-2.346196
C	-0.826527	-0.062898	-10.740581
H	-3.353829	-1.609986	-9.123050
H	0.961372	0.673400	-9.853665
H	-0.544215	0.335879	-11.716755
B	-2.041374	-1.192144	-6.687965
N	0.616373	-0.161920	-7.305966
C	2.028463	0.117248	-7.318075
C	2.928199	0.220227	-8.381978
C	2.493749	0.216174	-5.985970
C	4.273955	0.480134	-8.103030
C	3.830054	0.478294	-5.730631
C	4.747826	0.629102	-6.789290
H	2.629864	0.069521	-9.414853
H	4.973937	0.547723	-8.938551
H	4.180273	0.595521	-4.711737
C	6.162352	0.966309	-6.490566
C	6.871635	1.880631	-7.292095
C	6.810933	0.417998	-5.367246
C	8.177007	2.255113	-6.964667
C	8.117007	0.788553	-5.042512
C	8.802572	1.715216	-5.835746
H	6.382610	2.334513	-8.157543
H	6.287609	-0.312262	-4.746027
H	8.704920	2.979601	-7.590050
H	8.605648	0.345854	-4.170179
H	9.818401	2.020439	-5.571179
C	-2.987577	-0.931363	-11.719541
C	-2.496016	-1.080594	-13.031275
C	-4.383840	-0.962062	-11.530303
C	-3.365939	-1.232783	-14.112489
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C	-4.749164	-1.248458	-13.907971
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H	-2.957858	-1.346151	-15.120233
H	-6.333323	-1.121329	-12.436327
H	-5.429511	-1.362234	-14.755264
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C	-3.404829	-2.017709	-4.690824
C	-4.617768	-1.729864	-6.763322
C	-4.589769	-2.505490	-4.106637
H	-4.642822	-1.367233	-7.788438
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C	-5.759743	-2.590961	-4.845769
H	-4.601278	-2.822422	-3.065012
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C	-7.115411	-2.226826	-8.361487
C	-8.335979	-2.128662	-6.284015
C	-8.319167	-2.224963	-9.068113
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H	-10.480961	-2.181563	-8.940732
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C	-2.703654	-1.409998	-1.485672
C	-1.991736	-3.629263	-2.156103
C	-2.714490	-1.820210	-0.152404
C	-2.027681	-4.037847	-0.821737
C	-2.381780	-3.141428	0.204002
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H	-1.691679	-4.322983	-2.944629
H	-3.011322	-1.114836	0.626722
H	-1.753958	-5.063657	-0.565339
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C	-1.831556	-2.799773	2.634259
C	-3.051667	-4.784395	1.979858
C	-1.879838	-3.210697	3.967463
C	-3.111200	-5.188017	3.316144
C	-2.525862	-4.402138	4.313125
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H	-1.396401	-2.605573	4.737587
H	-3.625319	-6.115426	3.581603
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C	2.640847	2.173482	-2.909298
C	5.326019	1.519570	-2.256130
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H	6.354875	1.259290	-1.998265
H	3.384075	4.191546	-3.065690
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C	2.049204	-1.086514	-1.527212
C	2.187682	-2.478292	-1.622067
C	1.727133	-1.300274	0.862337
H	1.758657	0.586452	-0.186415
C	2.056201	-3.272140	-0.485916
H	2.384549	-2.932462	-2.595731
C	1.808819	-2.703275	0.780106
H	1.535113	-0.826768	1.827651
H	2.172893	-4.354541	-0.574433
C	1.617093	-3.552517	1.981075
C	0.881211	-4.749956	1.899602
C	2.129433	-3.164796	3.232917
C	0.654480	-5.528473	3.034832
H	0.444935	-5.052070	0.944622
C	1.908097	-3.947121	4.368514
H	2.725342	-2.252455	3.314842
C	1.166108	-5.129187	4.273750
H	0.054733	-6.438244	2.955439
H	2.323219	-3.630444	5.329166
H	0.981093	-5.735995	5.163555
H	5.731651	3.630543	-2.531257
C	1.246551	2.610525	-3.203334
C	1.004921	3.520998	-4.255025
C	0.141447	2.138177	-2.468352
C	-0.293655	3.928031	-4.572105
C	-1.156227	2.545067	-2.788276
C	-1.381861	3.435858	-3.843707
H	1.844393	3.887248	-4.850752
H	0.296261	1.438361	-1.646638
H	-0.457815	4.626455	-5.396441
H	-1.996887	2.165051	-2.202139
H	-2.397164	3.750876	-4.098114

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[3+H]+

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C	-1.194097	-0.909356	-5.567362
C	-2.170683	-0.450539	-10.509973
C	-0.371247	0.785998	-9.413123
C	1.022614	0.004385	-4.867241
C	-1.365541	-1.436980	-4.285022
C	-0.359206	-1.218027	-3.185525
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H	1.937058	0.521496	-5.125978
H	-0.847428	-0.649576	-2.376732
C	-1.096369	0.463417	-10.552473
H	-3.342773	-1.673121	-9.200232
H	0.463161	1.481350	-9.494712
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B	-2.239798	-1.134660	-6.647875
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C	1.412959	2.524576	-6.708066
C	2.478187	0.662596	-7.830191
C	2.627474	3.211074	-6.703488
C	3.679002	1.369390	-7.852985
C	3.791299	2.644797	-7.262191
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H	2.677842	4.187570	-6.218087
H	4.546709	0.916735	-8.335978
C	5.095416	3.355845	-7.213693
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C	5.162962	4.762275	-7.225522
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H	6.419231	6.515768	-7.197809
H	8.544385	5.214562	-7.080983
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C	-4.271744	-1.145921	-11.719926
C	-2.888566	-1.328001	-14.138728
C	-4.945216	-1.515848	-12.885344
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H	-6.016772	-1.729233	-12.846898
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C	-8.372924	-2.685288	-6.710093
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C	-3.207287	-1.879690	-1.620020
C	-1.980595	-3.866745	-2.262641
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C	-1.974827	-4.288322	-0.932588
C	-2.586039	-3.522585	0.080038
H	-3.693383	-0.941922	-1.900123
H	-1.492392	-4.462432	-3.037701
H	-3.737027	-1.723828	0.455312
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C	-2.510847	-3.032078	2.545456
C	-2.660940	-5.334423	1.826140
C	-2.539737	-3.445432	3.877267
C	-2.687718	-5.748193	3.159984
C	-2.631679	-4.804972	4.189956
H	-2.407679	-1.968866	2.316665
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N	1.891531	-0.408348	-2.675913
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C	3.146278	0.203092	-3.047106
C	3.416464	1.536582	-2.681834
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C	4.644934	2.093959	-3.077419
C	5.556217	1.366749	-3.845472
H	5.974297	-0.525549	-4.814419
H	4.868074	3.126056	-2.796229
C	0.879045	-0.232974	-0.430691
C	1.730759	-0.891376	-1.327384
C	2.408962	-2.046006	-0.918083
C	0.678030	-0.753082	0.847371
H	0.376439	0.686080	-0.737943
C	2.211757	-2.552629	0.366826
H	3.094045	-2.542264	-1.609076
C	1.332304	-1.925319	1.271000
H	-0.009258	-0.244623	1.527007
H	2.760987	-3.442523	0.681613
C	1.119855	-2.475922	2.633842
C	1.011378	-3.863523	2.841088
C	1.042398	-1.623940	3.751075
C	0.842951	-4.382722	4.125580
H	1.035609	-4.540251	1.983571
C	0.876027	-2.144464	5.037054
H	1.152108	-0.544722	3.614998
C	0.779592	-3.526211	5.228935
H	0.749692	-5.462187	4.265923
H	0.837541	-1.468094	5.894851
H	0.652808	-3.936093	6.234317
H	-0.091158	-2.167960	-2.697478
H	6.485514	1.838406	-4.173169
C	2.429822	2.356653	-1.922878
C	1.199931	2.719102	-2.500383
C	2.723790	2.791957	-0.621414
C	0.284420	3.498298	-1.788253
C	1.809287	3.574227	0.090144
C	0.586599	3.927804	-0.490327
H	0.968101	2.395160	-3.517374
H	3.671045	2.497012	-0.162238
H	-0.662169	3.786025	-2.254313

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C	-0.514143	2.006694	-7.621002
C	-0.014065	3.574268	-5.802184
C	-0.132114	3.284197	-7.154469
H	-1.196591	0.085548	-6.946426
H	0.319520	4.567094	-5.502719
C	-0.577772	0.541020	-2.813655
C	-0.541581	-0.509426	-1.855841
C	-0.007771	1.805396	-2.495020
C	0.037685	-0.290232	-0.592599
C	0.536866	2.023467	-1.213646
C	0.546738	0.974068	-0.294921
H	0.079737	-1.085259	0.150335
H	0.974825	2.981296	-0.939969
H	0.983378	1.149062	0.692703
C	-2.015626	-0.993763	-4.323103
C	-2.947129	-1.218831	-5.362820
C	-1.880173	-1.986728	-3.316827
C	-3.704357	-2.383306	-5.485737
C	-2.596545	-3.198680	-3.451832
C	-3.477659	-3.380877	-4.510440
H	-3.073123	-0.416310	-6.087431
H	-2.485464	-3.989622	-2.709348
N	0.023636	2.812733	-3.473893
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C	-0.492705	-2.910311	-1.521997
C	-1.079511	-3.481515	-0.393390
C	0.712990	-3.436728	-2.002902
C	-0.458554	-4.558498	0.255477
C	1.323934	-4.504125	-1.351545
C	0.759237	-5.088166	-0.200492
H	-2.015809	-3.066680	-0.012497
H	1.171642	-2.984429	-2.885276
H	-0.946056	-4.977076	1.135996
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C	0.594772	4.076841	-3.102430
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C	1.931517	4.363406	-3.405254
C	0.414501	6.225298	-1.997500
C	2.490094	5.580029	-3.019108
C	1.750846	6.536620	-2.295565
H	-1.200593	4.785625	-2.154659
H	2.522917	3.624881	-3.951311
H	-0.205422	6.925699	-1.437167
H	3.530622	5.783074	-3.282563
H	0.116434	4.074336	-7.868246
H	-4.019639	-4.328442	-4.566973
C	-0.487481	1.676569	-9.121835
C	0.942343	1.911034	-9.662389
H	1.670889	1.294961	-9.111961
H	1.002485	1.639334	-10.730236
H	1.251497	2.963595	-9.564326
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H	-2.508914	2.437435	-9.488104
H	-1.234919	3.652348	-9.746394
C	-0.857398	0.207805	-9.397050
H	-0.769067	-0.004123	-10.474770
H	-0.185777	-0.485398	-8.867360
H	-1.891045	-0.021930	-9.091551
C	-4.720453	-2.612525	-6.619848
C	-4.204303	-3.743999	-7.537646
H	-4.052805	-4.680937	-6.978947
H	-4.922713	-3.947974	-8.349649
H	-3.241184	-3.465816	-7.995671
C	-4.926948	-1.348406	-7.475746
H	-5.668255	-1.547660	-8.265858
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H	-3.997712	-1.026385	-7.971990
C	-6.093856	-3.014304	-6.033147
H	-6.825701	-3.166766	-6.844198
H	-6.042648	-3.950178	-5.455938
H	-6.480874	-2.228618	-5.365254
C	2.420537	7.855480	-1.869152
C	1.501768	-6.237947	0.506371
C	1.488311	8.725408	-1.008905
H	0.586842	9.030844	-1.563650
H	1.167399	8.199533	-0.095171
H	2.014218	9.642670	-0.699369
C	2.813946	8.659180	-3.130196
H	3.495603	8.088776	-3.779219
H	1.923611	8.921123	-3.724433
H	3.324723	9.594207	-2.845482
C	3.689260	7.543457	-1.042028
H	3.441035	6.935334	-0.157371
H	4.437359	6.990712	-1.630226
H	4.162797	8.477199	-0.695562
C	2.873881	-5.719783	1.003572
H	2.745200	-4.904866	1.733621
H	3.437598	-6.531660	1.493153
H	3.491605	-5.331473	0.178761
C	1.722493	-7.399703	-0.490007
H	2.328614	-7.089757	-1.355015
H	2.253619	-8.231451	0.001892
H	0.762836	-7.783203	-0.873076
C	0.724271	-6.780453	1.719020
H	-0.258838	-7.181975	1.425688
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H	0.565213	-6.005133	2.485089

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C	-0.425473	3.861479	-5.662788
C	-1.146519	3.854742	-6.843991
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H	0.055488	4.784087	-5.341636
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C	-0.022261	-0.623485	-2.127544
C	0.459481	1.696142	-2.748101
C	0.633815	-0.423841	-0.895923
C	1.113713	1.883570	-1.513353
C	1.185637	0.823090	-0.615455
H	0.716212	-1.226716	-0.166819
H	1.563038	2.838672	-1.251479
H	1.693648	0.976281	0.341058
C	-1.273513	-1.246462	-4.710995
C	-1.804249	-1.725634	-5.933128
C	-1.210280	-2.182784	-3.636349
C	-2.350326	-2.999217	-6.122594
C	-1.778197	-3.466183	-3.797673
C	-2.344277	-3.852014	-5.003829

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N	0.382183	2.754387	-3.659611
N	-0.587664	-1.868178	-2.419032
C	-0.371384	-2.933468	-1.479362
C	-1.259719	-3.160842	-0.428303
C	0.757481	-3.750130	-1.613595
C	-1.015645	-4.191836	0.486483
C	0.990983	-4.774844	-0.700091
C	0.112585	-5.022731	0.372991
H	-2.138919	-2.521210	-0.322568
H	1.448684	-3.569112	-2.439929
H	-1.728023	-4.331463	1.299614
H	1.882291	-5.392834	-0.828433
C	1.049288	3.980270	-3.313686
C	0.404583	4.943889	-2.537115
C	2.366708	4.203451	-3.727512
C	1.075599	6.113165	-2.162952
C	3.025112	5.375071	-3.355098
C	2.402814	6.354000	-2.556250
H	-0.621995	4.763711	-2.209807
H	2.869005	3.447882	-4.336128
H	0.541726	6.835255	-1.544631
H	4.054277	5.523354	-3.690119
H	-1.198224	4.778114	-7.426635
H	-2.777705	-4.850869	-5.061578
C	-2.634116	2.749248	-8.607532
C	-1.689413	3.162155	-9.707071
H	-0.988463	2.428411	-10.115605
H	-1.503447	4.218722	-9.920815
C	-3.777126	3.778554	-8.457959
H	-4.350226	3.858141	-9.396250
H	-4.465217	3.475491	-7.652951
H	-3.391098	4.779393	-8.208304
C	-3.254339	1.382548	-8.962725
H	-3.817022	1.460955	-9.905559
H	-2.484827	0.606292	-9.096336
H	-3.951733	1.044217	-8.181376
C	-2.929039	-3.418352	-7.487635
C	-1.813826	-3.364948	-8.555816
H	-0.982847	-4.036521	-8.287555
H	-2.205986	-3.676740	-9.538878
H	-1.400892	-2.349457	-8.663241
C	-4.072014	-2.459847	-7.891821
H	-4.504177	-2.760973	-8.861241
H	-4.878227	-2.473008	-7.141033
H	-3.719204	-1.422405	-7.991961
C	-3.497830	-4.848893	-7.461451
H	-3.908024	-5.105914	-8.451359
H	-2.723832	-5.593914	-7.218841
H	-4.315513	-4.953398	-6.730833
C	3.190453	7.607253	-2.131533
C	0.436881	-6.146033	1.374987
C	2.339079	8.566035	-1.282116
H	1.463746	8.936004	-1.839737
H	1.981245	8.086192	-0.357029
H	2.942202	9.440492	-0.990626
C	3.672781	8.372660	-3.385517
H	4.318988	7.751636	-4.023988
H	2.818477	8.709246	-3.994867
H	4.254468	9.261511	-3.090269
C	4.413492	7.167305	-1.292327
H	4.094124	6.598545	-0.404154
H	5.097245	6.527689	-1.871354
H	4.984749	8.046512	-0.950413
C	1.753368	-5.797653	2.109469
H	1.672480	-4.831340	2.632501
H	1.993715	-6.571814	2.856304
H	2.601058	-5.733160	1.409897
C	0.620299	-7.486751	0.625795
H	1.418433	-7.433280	-0.129657
H	0.893069	-8.284579	1.336268
H	-0.307715	-7.785313	0.111643
C	-0.676472	-6.326964	2.420780
H	-1.639336	-6.573187	1.944396
H	-0.421189	-7.153176	3.102829
H	-0.815853	-5.423786	3.035548

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B	-0.898557	0.274085	-4.347768
C	-0.960153	1.517296	-5.285429
C	-1.619672	1.546917	-6.538751
C	-0.345523	2.726573	-4.853551
C	-1.715626	2.670364	-7.358602
C	-0.420033	3.877084	-5.675052
C	-1.089818	3.843075	-6.888672
H	-2.098389	0.634147	-6.870493
H	0.040147	4.809883	-5.352109
C	-0.195683	0.503267	-3.009989
C	-0.093478	-0.548034	-2.054772
C	0.402984	1.760123	-2.699061
C	0.585653	-0.352186	-0.834268
C	1.079585	1.946113	-1.477100
C	1.154301	0.890224	-0.571237
H	0.671582	-1.153637	-0.103588
H	1.547576	2.896254	-1.229903
H	1.680654	1.045064	0.375026
C	-1.457397	-1.140966	-4.570270
C	-2.162627	-1.566541	-5.843316
C	-1.345994	-2.079083	-3.536877
C	-2.644414	-2.985549	-5.964912
C	-1.937226	-3.377807	-3.661136
C	-2.545508	-3.796482	-4.861056
H	-3.035558	-0.899554	-5.998721
H	-1.912551	-4.072157	-2.824417
N	0.326628	2.809512	-3.624360
N	-0.666821	-1.790885	-2.343540
C	-0.407104	-2.873083	-1.433873
C	-1.260797	-3.136013	-0.362859
C	0.721014	-3.679533	-1.626078
C	-0.990931	-4.198857	0.507049
C	0.983597	-4.733193	-0.753425
C	0.134143	-5.022916	0.332703
H	-2.139929	-2.505203	-0.213109
H	1.386112	-3.470012	-2.467044
H	-1.682868	-4.372375	1.331037
H	1.870518	-5.346027	-0.929540
C	1.005546	4.031932	-3.296130
C	0.381757	5.005321	-2.514582
C	2.319405	4.240383	-3.728976
C	1.071633	6.167070	-2.150801
C	2.996031	5.404734	-3.368704
C	2.396958	6.390225	-2.560732
H	-0.642320	4.836724	-2.173698
H	2.804448	3.477736	-4.342754
H	0.555204	6.896005	-1.525771
H	4.021954	5.541031	-3.718406
H	-1.129379	4.762113	-7.479764
H	-2.928861	-4.818137	-4.889974
C	-2.494334	2.680391	-8.685214
C	-1.576281	3.141882	-9.838931
H	-0.721197	2.456891	-9.956919
H	-2.134319	3.159596	-10.790368

H	-1.173028	4.152608	-9.669784
C	-3.686781	3.655073	-8.549132
H	-4.256399	3.712583	-9.492196
H	-4.371456	3.319856	-7.753791
H	-3.349560	4.671515	-8.291001
C	-3.049952	1.291117	-9.048784
H	-3.594522	1.339968	-10.005334
H	-2.244121	0.549296	-9.161393
H	-3.753840	0.921084	-8.287970
C	-3.168057	-3.474872	-7.316856
C	-1.949926	-3.865574	-8.193550
H	-1.364815	-4.664429	-7.711184
H	-2.283902	-4.229054	-9.180615
H	-1.280831	-3.006321	-8.359485
C	-3.969033	-2.369774	-8.037822
H	-4.389774	-2.760544	-8.978607
H	-4.806267	-2.011424	-7.417186
H	-3.340410	-1.504959	-8.295045
C	-4.080701	-4.707105	-7.165161
H	-4.478467	-5.008837	-8.147719
H	-3.541969	-5.573655	-6.752653
H	-4.934564	-4.489376	-6.503896
C	3.207724	7.632494	-2.148179
C	0.482499	-6.184313	1.281922
C	2.388245	8.594513	-1.271132
H	1.503186	8.978179	-1.803727
H	2.048329	8.110604	-0.341513
H	3.007644	9.460426	-0.988319
C	3.664514	8.398952	-3.410816
H	4.284353	7.772647	-4.070081
H	2.797565	8.748894	-3.994153
H	4.265400	9.279028	-3.127490
C	4.448490	7.176695	-1.343461
H	4.147751	6.602081	-0.452541
H	5.113366	6.537770	-1.944879
H	5.034405	8.048722	-1.007997
C	1.809834	-5.857210	2.008544
H	1.725910	-4.920036	2.581648
H	2.074887	-6.665239	2.709902
H	2.642653	-5.742819	1.297811
C	0.655130	-7.491598	0.474589
H	1.440084	-7.404853	-0.291965
H	0.941683	-8.317641	1.146226
H	-0.281407	-7.770421	-0.035025
C	-0.610006	-6.414994	2.339868
H	-1.579472	-6.651855	1.872403
H	-0.334522	-7.264464	2.984680
H	-0.746471	-5.537642	2.991511
H	-1.512358	-1.327091	-6.708133

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B	-1.162873	0.285784	-4.217285
C	-0.831183	1.353362	-5.269090
C	-0.926493	1.135284	-6.657573
C	-0.296822	2.599135	-4.821220
C	-0.580303	2.090348	-7.611523
C	-0.076693	3.632646	-5.771277
C	-0.214584	3.371720	-7.121683
H	-1.242753	0.147934	-6.984085
H	0.243285	4.621783	-5.448288
C	-0.551365	0.523113	-2.854361
C	-0.474813	-0.539484	-1.920874
C	0.018429	1.780170	-2.528662
C	0.142819	-0.334945	-0.657619
C	0.586989	1.987816	-1.241707
C	0.634208	0.929238	-0.335803
H	0.221162	-1.149781	0.060312
H	1.010177	2.951881	-0.966079
H	1.086262	1.092439	0.645010
C	-1.987338	-1.005137	-4.352932
C	-2.922182	-1.243046	-5.381183
C	-1.809476	-2.013588	-3.358093
C	-3.648372	-2.428242	-5.503868
C	-2.487521	-3.251940	-3.500313
C	-3.378094	-3.438544	-4.543015
H	-3.083102	-0.441408	-6.098521
H	-2.337687	-4.049822	-2.773719
N	0.051890	2.793318	-3.480485
N	-0.981828	-1.790963	-2.251389
C	-0.455790	-2.934206	-1.530669
C	-1.091770	-3.476051	-0.415816
C	0.756856	-3.471678	-1.975696
C	-0.501534	-4.553304	0.260026
C	1.331413	-4.539420	-1.293427
C	0.723094	-5.104154	-0.154600
H	-2.035280	-3.049536	-0.066631
H	1.247777	-3.039613	-2.850870
H	-1.019173	-4.957109	1.129592
H	2.280447	-4.937667	-1.657536
C	0.628460	4.065118	-3.098493
C	-0.132625	4.994289	-2.392117
C	1.958863	4.347948	-3.425374
C	0.445217	6.207189	-2.000892
C	2.514479	5.566943	-3.044667
C	1.777099	6.523459	-2.317046
H	-1.169264	4.764557	-2.134310
H	2.547627	3.613540	-3.980053
H	-0.170601	6.908952	-1.438667
H	3.550578	5.774112	-3.319116
H	0.003210	4.178996	-7.824211
H	-3.895901	-4.397498	-4.608957
C	-0.556549	1.791583	-9.113939
C	0.873565	2.057144	-9.643543
H	1.611114	1.440396	-9.106183
H	0.933462	1.802599	-10.714188
H	1.168273	3.112305	-9.533016
C	-1.568703	2.710911	-9.833155
H	-1.567166	2.508240	-10.916378
H	-2.589636	2.542646	-9.453887
H	-1.327872	3.776579	-9.694906
C	-0.910187	0.324610	-9.417788
H	-0.822231	0.139146	-10.499164
H	-0.226885	-0.373488	-8.909443
H	-1.941845	0.076175	-9.119366
C	-4.670215	-2.669086	-6.624360
C	-4.118797	-3.767447	-7.563814
H	-3.927351	-4.709419	-7.026716
H	-4.842230	-3.980500	-8.367142
H	-3.174622	-3.445525	-8.032155
C	-4.930122	-1.398275	-7.455598
H	-5.679719	-1.610822	-8.232663
H	-5.319562	-0.577217	-6.833010
H	-4.022770	-1.042431	-7.969476
C	-6.017875	-3.129182	-6.019471
H	-6.752972	-3.288301	-6.824402
H	-5.929910	-4.076182	-5.465891
H	-6.423864	-2.370432	-5.332343
C	2.442545	7.848500	-1.908731
C	1.426407	-6.256955	0.583106
C	1.512037	8.720442	-1.049129
H	0.604837	9.018365	-1.598698
H	1.203796	8.204749	-0.125202
H	2.035820	9.642824	-0.754552

C	2.818196	8.638332	-3.184571
H	3.502451	8.069419	-3.832302
H	1.921604	8.888638	-3.774158
H	3.321969	9.579705	-2.912307
C	3.720815	7.546632	-1.091952
H	3.485850	6.946033	-0.198534
H	4.469390	6.997126	-1.682743
H	4.189624	8.486090	-0.757796
C	2.783560	-5.744116	1.125603
H	2.636366	-4.928603	1.851408
H	3.321677	-6.559610	1.635371
H	3.435019	-5.365088	0.322578
C	1.672052	-7.422733	-0.403250
H	2.314902	-7.125262	-1.245784
H	2.176337	-8.255379	0.112614
H	0.724057	-7.801710	-0.818183
C	0.598455	-6.785934	1.767524
H	-0.376604	-7.180725	1.440108
H	1.140064	-7.608446	2.259224
H	0.421230	-6.008799	2.527836

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B	-0.545181	0.239466	-4.915612
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C	-1.704459	1.459569	-6.890769
C	-0.281462	2.767052	-5.424346
C	-2.121385	2.583454	-7.601375
C	-0.704780	3.917604	-6.113926
C	-1.595144	3.820103	-7.176388
H	-2.127052	0.496868	-7.154546
H	-0.381014	4.906055	-5.808455
C	0.230840	0.549840	-3.650921
C	0.305106	-0.333958	-2.541412
C	0.832031	1.795168	-3.514035
C	0.911393	0.111668	-1.283225
C	1.780160	2.130780	-2.419044
C	1.552769	1.298609	-1.196143
H	0.823058	-0.525249	-0.403823
H	2.773299	1.777764	-2.792486
H	2.009410	1.615122	-0.254813
C	-1.033169	-1.230239	-4.996353
C	-1.618244	-1.841882	-6.126836
C	-0.920469	-2.028334	-3.816023
C	-2.153196	-3.135217	-6.136832
C	-1.469697	-3.324261	-3.797344
C	-2.077738	-3.853027	-4.928242
H	-1.644359	-1.269682	-7.052950
H	-1.428894	-3.933751	-2.897330
N	0.611155	2.859058	-4.315709
N	-0.271114	-1.551615	-2.635243
C	-0.208606	-2.457674	-1.502993
C	-1.232374	-2.471577	-0.556329
C	0.855586	-3.359373	-1.405502
C	-1.201812	-3.411601	0.479705
C	0.869197	-4.292201	-0.369944
C	-0.165921	-4.357735	0.585422
H	-2.061125	-1.763920	-0.638065
H	1.650965	-3.346055	-2.154602
H	-2.017739	-3.399432	1.202043
H	1.700219	-4.998555	-0.318922
C	1.281086	4.010184	-3.739096
C	1.870213	3.630928	-2.513755
C	1.463598	5.314553	-4.197776
C	2.552232	4.539677	-1.721054
C	2.153657	6.224701	-3.381941
C	2.690445	5.883737	-2.129748
H	1.122692	5.655010	-5.170956
H	2.991797	4.200523	-0.781041
H	2.271225	7.238087	-3.764482
H	-1.902077	4.743143	-7.673264
H	-2.492030	-4.858018	-4.854993
C	-3.132688	2.516468	-8.757075
C	-2.479046	3.082076	-10.039160
H	-1.602895	2.481354	-10.331118
H	-3.198281	3.059996	-10.873534
H	-2.143961	4.123777	-9.912810
C	-4.378653	3.351472	-8.377853
H	-5.110543	3.343132	-9.201478
H	-4.868418	2.934143	-7.483184
H	-4.128051	4.402202	-8.163316
C	-3.594000	1.075033	-9.045967
H	-4.315244	1.074568	-9.877479
H	-2.755372	0.423509	-9.338449
H	-4.098385	0.624693	-8.176476
C	-2.800472	-3.713948	-7.408134
C	-1.765175	-3.708636	-8.555743
H	-0.886762	-4.321224	-8.297877
H	-2.213981	-4.124349	-9.472191
H	-1.410977	-2.692321	-8.790159
C	-4.016417	-2.845258	-7.806570
H	-4.499409	-3.261333	-8.705389
H	-4.766025	-2.820491	-6.999710
H	-3.725430	-1.808547	-8.036591
C	-3.289335	-5.160298	-7.202455
H	-3.739145	-5.535547	-8.134518
H	-2.464596	-5.839793	-6.936034
H	-4.061446	-5.229004	-6.420065
C	3.401608	6.899032	-1.216123
C	-0.134572	-5.449158	1.670941
C	2.493182	7.174502	0.005504
H	1.541929	7.633367	-0.308723
H	2.258557	6.249836	0.557099
H	2.991820	7.866386	0.703486
C	3.676370	8.236198	-1.931888
H	4.309945	8.102158	-2.823104
H	2.747907	8.742527	-2.239444
H	4.205706	8.918640	-1.249385
C	4.753971	6.321666	-0.734509
H	4.628632	5.435311	-0.093636
H	5.394211	6.039249	-1.585501
H	5.292956	7.073325	-0.136646
C	1.140321	-5.283517	2.529415
H	1.181063	-4.286938	2.997615
H	1.155875	-6.035861	3.333735
H	2.055398	-5.420745	1.932252
C	-0.113882	-6.838703	0.992220
H	0.773087	-6.977691	0.355207
H	-0.098273	-7.630686	1.758360
H	-1.007551	-6.989333	0.365854
C	-1.366955	-5.383840	2.588951
H	-2.300319	-5.542763	2.024734
H	-1.304178	-6.173535	3.352996
H	-1.437875	-4.421383	3.120343

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[4+H]+

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B	-0.803126	0.213151	-4.465971
C	-0.910751	1.478885	-5.355185
C	-1.629827	1.548716	-6.571776
C	-0.288106	2.675798	-4.911398
C	-1.730593	2.692840	-7.361018
C	-0.354018	3.844104	-5.700054
C	-1.053659	3.841753	-6.896639

H	-2.155604	0.658093	-6.892973
H	0.130349	4.761366	-5.370749
C	-0.148176	0.446651	-3.100489
C	-0.077757	-0.596047	-2.149973
C	0.435397	1.710529	-2.777888
C	0.571026	-0.405217	-0.803476
C	1.107882	1.923113	-1.499718
C	1.166397	0.938610	-0.587638
H	-0.171844	-0.605272	-0.008674
H	1.563857	2.886270	-1.284645
H	1.669193	1.111688	0.367778
C	-1.308188	-1.233640	-4.717667
C	-1.864898	-1.723596	-5.922847
C	-1.262265	-2.147423	-3.628524
C	-2.450982	-2.985508	-6.065917
C	-1.859323	-3.416631	-3.737344
C	-2.457018	-3.811260	-4.925325
H	-1.824003	-1.082656	-6.800559
H	-1.866244	-4.101884	-2.891805
N	0.387068	2.735244	-3.661901
N	-0.605496	-1.811750	-2.413270
C	-0.376599	-2.887664	-1.466964
C	-1.241051	-3.103380	-0.395913
C	0.735314	-3.716279	-1.652020
C	-0.976320	-4.140151	0.507129
C	0.984206	-4.744864	-0.747212
C	0.139687	-4.982693	0.355944
H	-2.119403	-2.466336	-0.265293
H	1.395941	-3.553627	-2.507180
H	-1.666756	-4.280240	1.338270
H	1.857936	-5.378418	-0.910019
C	1.042113	3.983398	-3.309003
C	0.363277	4.935421	-2.550567
C	2.365186	4.206196	-3.698582
C	1.024449	6.100922	-2.148940
C	3.008308	5.376477	-3.295929
C	2.364177	6.343933	-2.498522
H	-0.672839	4.754991	-2.254155
H	2.887719	3.460489	-4.302701
H	0.473371	6.818401	-1.541249
H	4.044437	5.531124	-3.603393
H	-1.086579	4.767542	-7.474995
H	-2.920615	-4.796608	-4.955738
C	-2.546059	2.745626	-8.662247
C	-1.616430	3.123385	-9.837881
H	-0.817093	2.376470	-9.967554
H	-2.194061	3.169417	-10.775227
H	-1.139369	4.105298	-9.693183
C	-3.654378	3.813241	-8.509265
H	-4.249809	3.881104	-9.433731
H	-4.335420	3.557900	-7.681947
H	-3.236902	4.811637	-8.305244
C	-3.215937	1.398032	-8.988723
H	-3.783554	1.482072	-9.927949
H	-2.476977	0.592548	-9.124530
H	-3.924335	1.092256	-8.203690
C	-3.049611	-3.430549	-7.412277
C	-1.920498	-3.481359	-8.466598
H	-1.128490	-4.184325	-8.164004
H	-2.321594	-3.816104	-9.437148
H	-1.455785	-2.493804	-8.616372
C	-4.134062	-2.426301	-7.865221
H	-4.582219	-2.757858	-8.815808
H	-4.940543	-2.350815	-7.118692
H	-3.723706	-1.418123	-8.029082
C	-3.698716	-4.823314	-7.322541
H	-4.119388	-5.100054	-8.301527
H	-2.970172	-5.601239	-7.045835
H	-4.525160	-4.845910	-6.594665
C	3.140027	7.586322	-2.026219
C	0.484351	-6.111488	1.342667
C	2.266995	8.523821	-1.174922
H	1.408549	8.913547	-1.745145
H	1.885662	8.022458	-0.270630
H	2.864447	9.387718	-0.845554
C	3.654328	8.376310	-3.251921
H	4.320676	7.771217	-3.885280
H	2.817766	8.728770	-3.876287
H	4.226505	9.257131	-2.919447
C	4.341319	7.121501	-1.168405
H	4.001219	6.537106	-0.298100
H	5.040724	6.495815	-1.744214
H	4.903852	7.992469	-0.795297
C	1.832114	-5.776613	2.026289
H	1.783915	-4.810410	2.553714
H	2.085687	-6.553716	2.764158
H	2.656897	-5.727769	1.298314
C	0.624772	-7.450386	0.580696
H	1.398852	-7.407737	-0.200224
H	0.911696	-8.251461	1.280444
H	-0.323960	-7.738343	0.099507
C	-0.593312	-6.278858	2.427107
H	-1.575675	-6.516570	1.987542
H	-0.322404	-7.108310	3.097830
H	-0.698237	-5.376277	3.049814
H	1.336636	-1.183784	-0.628927

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C	-2.646969	2.348507	-5.939372
C	-3.603999	2.386552	-6.954619
C	-1.296713	2.341654	-6.313955
H	-2.943467	2.319255	-4.889823
C	-3.234292	2.413607	-8.313493
H	-4.663622	2.393927	-6.684042
C	-0.908669	2.356935	-7.682035
C	-1.889429	2.395572	-8.682488
H	-4.009885	2.445727	-9.082641
C	0.538395	2.308655	-7.706533
H	-1.597686	2.407480	-9.736280
C	0.969867	2.269714	-6.352424
C	2.331326	2.242009	-6.021552
C	1.486539	2.299855	-8.738936
C	3.255208	2.234621	-7.067538
H	2.660346	2.229287	-4.981262
C	2.842154	2.258420	-8.414100
H	1.161612	2.326276	-9.782658
H	3.592555	2.246865	-9.208397
H	4.322794	2.210276	-6.831575
N	-0.149908	2.291765	-5.516911
C	-0.847663	3.069667	-1.928272
C	-0.823574	3.151126	-3.320206
C	-0.126113	2.036944	-1.315512
H	-1.405981	3.795644	-1.335601
C	-0.127158	2.200036	-4.100119
H	-1.351671	3.960865	-3.826984
C	0.601345	1.089325	-2.087225
C	0.578856	1.161594	-3.483345
C	1.219447	0.171180	-1.153002
H	1.098303	0.417750	-4.090388
C	0.827132	0.589848	0.147207
C	1.282863	-0.069143	1.296223
C	2.073194	-0.931667	-1.301115
C	2.135275	-1.161235	1.122270

H	0.987072	0.268683	2.291026
C	2.527494	-1.593121	-0.160575
H	2.384438	-1.263117	-2.295688
H	3.194246	-2.453038	-0.261271
H	2.509993	-1.691658	2.001786
N	0.009343	1.718579	0.037117
C	-1.484682	1.656098	1.969173
C	-2.106474	2.312368	3.033300
C	-0.638409	2.378566	1.115141
C	-1.906195	3.678819	3.238156
C	-0.429759	3.746444	1.327000
C	-1.067453	4.420802	2.383832
H	-2.771875	1.755564	3.697884
H	-2.428638	4.184416	4.052800
H	0.262272	4.280950	0.673444
C	-0.855107	5.877246	2.593397
C	-0.780338	6.419110	3.890839
C	-0.734515	6.755465	1.499346
C	-0.601514	7.789779	4.087937
C	-0.557956	8.126430	1.695920
C	-0.493812	8.650237	2.991070
H	-0.843381	5.754982	4.756180
H	-0.806963	6.363310	0.481592
H	-0.538539	8.189692	5.103780
H	-0.476002	8.790140	0.831260
H	-0.354606	9.723359	3.146345
H	-1.655729	0.593872	1.783233

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C	-2.742868	1.969172	-6.026599
C	-3.704986	1.942201	-7.037268
C	-1.397064	2.062057	-6.406707
H	-3.032778	1.915732	-4.976160
C	-3.344447	1.997560	-8.397689
H	-4.761026	1.872920	-6.761561
C	-1.017695	2.102606	-7.776466
C	-2.003212	2.072103	-8.772521
H	-4.123992	1.976441	-9.163170
C	0.428711	2.162337	-7.807745
H	-1.717671	2.104895	-9.827529
C	0.868654	2.163531	-6.455753
C	2.229662	2.249037	-6.133045
C	1.368898	2.223135	-8.845483
C	3.145722	2.307676	-7.184303
H	2.565359	2.273791	-5.095226
C	2.725247	2.289921	-8.528513
H	1.036868	2.221078	-9.887267
H	3.469753	2.335487	-9.327058
H	4.212823	2.372522	-6.954084
N	-0.246026	2.101069	-5.614907
C	-1.016407	3.007953	-2.077245
C	-0.998244	3.009043	-3.470031
C	-0.202395	2.083194	-1.412599
H	-1.631250	3.718621	-1.522757
C	-0.215282	2.082160	-4.195952
H	-1.595576	3.737681	-4.020517
C	0.623153	1.172258	-2.124765
C	0.591649	1.156993	-3.523851
C	1.359432	0.413490	-1.132777
H	1.188627	0.439429	-4.089609
C	0.942167	0.893226	0.139970
C	1.448863	0.358087	1.329806
C	2.316681	-0.608703	-1.206374
C	2.400442	-0.659354	1.227858
H	1.104116	0.726792	2.298198
C	2.835612	-1.137925	-0.024493
H	2.651240	-0.985728	-2.176807
H	3.583568	-1.933506	-0.068346
H	2.817333	-1.096625	2.139288
N	-0.006678	1.901475	-0.044480
C	-2.114467	2.435732	1.066858
C	-2.737743	3.183041	2.040147
C	-0.716383	2.600447	0.965766
C	-2.130208	4.063094	2.906920
C	-0.039536	3.465998	1.833985
C	-0.724727	4.215600	2.809680
H	-2.705143	4.664464	3.615406
H	1.043129	3.555160	1.731453
C	-0.012684	5.196289	3.671374
C	-0.433444	5.445696	4.991733
C	1.077741	5.934469	3.171436
C	0.204892	6.407680	5.777776
C	1.720339	6.891561	3.959427
C	1.283860	7.135843	5.265332
H	1.409483	5.780243	2.141933
H	-0.144786	6.591813	6.797436
H	2.556084	7.460803	3.543858
H	1.781250	7.889117	5.881483
H	-2.637813	1.747014	0.398958
H	-1.258667	4.866810	5.413894

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C	-2.652994	2.370665	-5.915368
C	-3.590935	2.409521	-6.948072
C	-1.296337	2.414099	-6.263000
H	-2.968703	2.301988	-4.873358
C	-3.195944	2.485120	-8.297922
H	-4.655272	2.378239	-6.698592
C	-0.882160	2.480746	-7.621755
C	-1.844296	2.517559	-8.640273
H	-3.957162	2.515547	-9.081308
C	0.566159	2.477593	-7.617762
H	-1.533061	2.567792	-9.687268
C	0.971551	2.414549	-6.256557
C	2.326038	2.424167	-5.897163
C	1.535377	2.524621	-8.629322
C	3.271101	2.471756	-6.922804
H	2.633301	2.396534	-4.850439
C	2.884779	2.515762	-8.276790
H	1.231466	2.568975	-9.678737
H	3.651257	2.548207	-9.054975
H	4.333873	2.476711	-6.664765
N	-0.164400	2.375957	-5.444471
C	-0.970305	2.932022	-1.839198
C	-0.913963	3.094182	-3.222980
C	-0.224430	1.894234	-1.266012
H	-1.579968	3.597842	-1.226128
C	-0.167523	2.210710	-4.034609
H	-1.458970	3.911612	-3.698395
C	0.551166	1.012502	-2.068779
C	0.556445	1.160904	-3.458609
C	1.176956	0.065086	-1.168708
H	1.112157	0.467995	-4.093208
C	0.742592	0.404191	0.141270
C	1.190775	-0.296205	1.267821
C	2.068564	-1.002675	-1.349372
C	2.085839	-1.348104	1.061946
H	0.850590	-0.021725	2.268123
C	2.520494	-1.703074	-0.231023
H	3.218878	-2.534002	-0.357730
H	2.457989	-1.909736	1.923006
N	-0.114248	1.508729	0.069321

C	-1.640862	1.528614	1.949689
C	-2.154403	2.155952	3.118380
C	-0.704245	2.160619	1.181434
C	-1.674978	3.413825	3.522484
C	-0.182303	3.530102	1.520773
C	-0.715798	4.122812	2.807863
H	-2.909814	1.644995	3.718755
H	-2.074782	3.831614	4.447871
H	0.925007	3.469126	1.550795
C	-0.169963	5.409751	3.258868
C	-0.644296	6.062490	4.424475
C	0.877201	6.048763	2.551340
C	-0.087748	7.258149	4.868017
C	1.438550	7.245622	3.000701
C	0.966280	7.857180	4.164580
H	-1.463021	5.626768	4.998683
H	1.279134	5.603780	1.640600
H	-0.481799	7.731551	5.771509
H	2.252706	7.703444	2.432223
H	1.412502	8.788485	4.523012
H	-1.985811	0.533932	1.656900
H	2.412470	-1.276196	-2.350785
H	-0.380914	4.229202	0.680274

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C	-2.677142	2.413664	-5.953770
C	-3.629369	2.485966	-6.974702
C	-1.327658	2.369818	-6.327566
H	-2.989368	2.374113	-4.910310
C	-3.248184	2.496067	-8.325929
H	-4.688716	2.526423	-6.710918
C	-0.932908	2.353043	-7.690260
C	-1.896765	2.419747	-8.693491
H	-4.015757	2.550354	-9.101044
C	0.517358	2.219277	-7.713982
H	-1.604983	2.400497	-9.746135
C	0.949894	2.153191	-6.364840
C	2.309593	2.105082	-6.029474
C	1.453092	2.186167	-8.745269
C	3.233382	2.067288	-7.077998
H	2.649400	2.119034	-4.993657
C	2.814299	2.098267	-8.417759
H	1.132899	2.240085	-9.788360
H	3.559985	2.070151	-9.215335
H	4.299976	2.024776	-6.845590
N	-0.176655	2.241531	-5.523337
C	-0.946638	3.019486	-1.975064
C	-0.941283	3.077024	-3.358300
C	-0.150307	2.039830	-1.346808
H	-1.536808	3.721930	-1.385861
C	-0.153694	2.174712	-4.128566
H	-1.511236	3.852503	-3.870453
C	0.650124	1.126440	-2.110471
C	0.647193	1.195433	-3.492918
C	1.304581	0.248173	-1.155500
H	1.205764	0.473035	-4.089201
C	0.876999	0.666996	0.129592
C	1.347231	0.067630	1.299963
C	2.209540	-0.810352	-1.274639
C	2.254507	-0.989236	1.158406
H	1.025322	0.418416	2.281671
C	2.678144	-1.427189	-0.108085
H	2.550939	-1.151886	-2.255203
H	3.383856	-2.257459	-0.183446
H	2.644533	-1.482256	2.051988
N	-0.011930	1.749727	-0.014184
C	-1.522625	1.665657	1.903062
C	-2.165278	2.319072	2.956401
C	-0.683357	2.408545	1.061591
C	-1.978340	3.687824	3.160316
C	-0.486977	3.778591	1.264047
C	-1.138399	4.444725	2.317967
H	-2.831870	1.757574	3.614927
H	-2.511198	4.186478	3.972152
H	0.208275	4.320834	0.620067
C	-0.939570	5.900437	2.536421
C	-0.877367	6.432614	3.838393
C	-0.819923	6.783668	1.446337
C	-0.708256	7.803139	4.043145
C	-0.655728	8.154547	1.651520
C	-0.601515	8.669475	2.950722
H	-0.940329	5.764730	4.700806
H	-0.886940	6.398043	0.425380
H	-0.653690	8.198482	5.060769
H	-0.576967	8.825571	0.792562
H	-0.472683	9.742579	3.112835
H	-1.678818	0.601230	1.716439

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C	-2.947460	3.204493	-6.817323
C	-3.356906	3.593964	-8.098697
C	-1.748790	2.506278	-6.713333
H	-3.549343	3.448805	-5.941221
C	-2.589198	3.283013	-9.230920
H	-4.290784	4.148088	-8.215951
C	-0.943486	2.181205	-7.856240
C	-1.383668	2.577755	-9.119724
H	-2.941089	3.601056	-10.215317
C	0.256372	1.462971	-7.383720
H	-0.794299	2.339827	-10.007758
C	0.096938	1.419386	-6.009155
C	0.884353	0.872594	-5.021447
C	1.432604	0.846049	-7.839511
C	2.038952	0.234403	-5.494705
C	2.288574	0.250289	-6.887045
H	1.700742	0.810444	-8.897846
H	3.198762	-0.234361	-7.248280
H	2.742390	-0.273967	-4.834687
N	-1.081183	2.008676	-5.563536
C	-1.711755	2.455790	-1.951322
C	-2.039748	2.474897	-3.310747
C	-0.485334	1.929142	-1.502443
H	-2.388133	2.918009	-1.228640
C	-1.142314	1.910736	-4.219833
H	-2.932428	2.997470	-3.653948
C	0.479842	1.360854	-2.368745
C	0.044889	1.045790	-3.759720
C	1.631717	1.084977	-1.598928
H	-0.455045	0.050708	-3.639034
C	1.322481	1.488145	-0.252862
C	2.254785	1.350815	0.789783
C	2.921831	0.568515	-1.887208
C	3.503405	0.840687	0.466748
H	2.001363	1.640878	1.810123
C	3.840320	0.461173	-0.861657
H	3.186292	0.267760	-2.900518
H	4.838867	0.069331	-1.067267
H	4.250448	0.723533	1.255428
N	0.037210	1.984967	-0.213165
C	-1.814475	1.863999	1.386724
C	-2.435203	2.343610	2.543847
C	-0.632937	2.477666	0.952183

C	-1.873982	3.400898	3.263435
C	-0.072897	3.542549	1.665072
C	-0.676418	4.013031	2.844645
H	-3.358623	1.877176	2.896039
H	-2.377564	3.772133	4.158574
H	0.860305	3.985936	1.313173
C	-0.049726	5.108064	3.629755
C	-0.042208	5.064746	5.037108
C	0.574540	6.196015	2.989840
C	0.580906	6.071606	5.777652
C	1.194240	7.204821	3.731162
C	1.202362	7.144525	5.129096
H	-0.497948	4.218869	5.558077
H	0.554008	6.267173	1.899066
H	0.590387	6.010685	6.869004
H	1.666234	8.044150	3.214006
H	1.689557	7.929875	5.712148
H	-2.225744	1.015413	0.835070
C	-1.002749	4.385913	2.405237
H	-2.858479	1.774050	3.624098
H	-2.397739	4.171291	4.046523
H	0.349851	4.225373	0.715028
C	-0.728551	5.824722	2.655606
C	-0.628594	6.322995	3.968377
C	-0.578460	6.727621	1.585999
C	-0.396036	7.679351	4.203719
C	-0.349956	8.084552	1.821393
C	-0.260804	8.566348	3.131338
H	-0.714556	5.636957	4.814467
H	-0.672363	6.367653	0.557685
H	-0.314192	8.047344	5.229908
H	-0.247661	8.771355	0.977285
H	-0.081210	9.628329	3.317127
H	-1.766384	0.604379	1.697297
H	3.407102	1.411798	-8.794608

[Host+H]+

C	-2.657772	2.317084	-5.960174
C	-3.608681	2.349288	-6.987396
C	-1.319199	2.337107	-6.341583
H	-2.956057	2.272368	-4.912534
C	-3.227871	2.389802	-8.338830
H	-4.669869	2.338949	-6.727377
C	-0.917282	2.368156	-7.694023
C	-1.878335	2.394234	-8.706258
H	-3.997702	2.413572	-9.113056
C	0.541084	2.340238	-7.692225
H	-1.584421	2.415010	-9.758415
C	0.942078	2.310522	-6.289862
C	2.316766	2.322311	-5.889133
C	1.485969	2.327584	-8.665264
C	3.262868	2.313117	-6.862247
H	2.582524	2.341722	-4.831779
C	2.931669	2.294650	-8.315369
H	1.203212	2.339565	-9.722165
H	3.451527	3.137641	-8.817687
H	4.321540	2.326050	-6.586865
N	-0.151573	2.296697	-5.518368
C	-0.888559	3.035509	-1.932418
C	-0.875814	3.126134	-3.321374
C	-0.160602	1.998804	-1.327040
H	-1.439690	3.757990	-1.329448
C	-0.160942	2.182817	-4.091957
H	-1.405679	3.939699	-3.820159
C	0.570106	1.046581	-2.105112
C	0.551219	1.134027	-3.495839
C	1.192512	0.131782	-1.173921
H	1.067500	0.391898	-4.108834
C	0.806845	0.560527	0.123335
C	1.262214	-0.088026	1.277259
C	2.045751	-0.973335	-1.319431
C	2.112426	-1.181056	1.106719
H	0.966268	0.257184	2.269113
C	2.501482	-1.623489	-0.174888
H	2.353356	-1.317458	-2.310829
H	3.165963	-2.485439	-0.268528
H	2.489084	-1.706833	1.987606
N	-0.017227	1.688043	0.009830
C	-1.549180	1.652687	1.912602
C	-2.156693	2.312828	2.983029
C	-0.656276	2.359099	1.096600
C	-1.889740	3.661553	3.225557
C	-0.379449	3.707736	1.341685

[1–H]+_os

C	-2.527741	-1.615377	-9.288930
C	-1.901230	-0.902896	-8.248548
C	-0.701189	-0.187282	-8.566701
C	-0.233946	0.353831	-6.214496
C	-1.368842	-0.377272	-5.775283
C	-2.065403	-1.625751	-10.611202
C	-0.239934	-0.156410	-9.909370
C	0.615561	0.986737	-5.266717
C	-1.573039	-0.550810	-4.381309
C	-0.688572	0.038807	-3.444046
C	0.373962	0.813750	-3.905918
H	1.450694	1.604921	-5.588702
H	-0.848723	-0.085368	-2.374166
H	1.033688	1.299109	-3.183608
C	-0.911608	-0.851072	-10.896866
H	-3.383966	-2.241677	-9.040229
H	0.657281	0.402886	-10.169203
H	-0.536263	-0.798046	-11.921354
B	-2.363930	-0.931808	-6.776088
N	0.041978	0.455836	-7.574025
C	1.224146	1.190870	-7.959075
C	1.138032	2.516309	-8.416943
C	2.496341	0.662305	-7.838566
C	2.300690	3.239342	-8.688554
C	3.669544	1.331913	-8.086333
C	3.585519	2.681787	-8.515635
H	0.154146	2.978831	-8.535230
H	2.211369	4.278059	-9.012405
H	4.642176	0.845071	-7.975474
C	4.814478	3.481033	-8.751165
C	5.928345	3.345798	-7.899183
C	4.889024	4.402256	-9.814307
C	7.078705	4.111299	-8.100982
C	6.042651	5.162679	-10.018854
C	7.139765	5.021598	-9.162283
H	5.884027	2.657289	-7.051265
H	4.045698	4.511572	-10.500934
H	7.929141	3.997322	-7.423660
H	6.088985	5.863936	-10.855873
H	8.041568	5.616901	-9.326274
C	-2.739080	-2.435834	-11.650774
C	-1.999749	-3.077395	-12.666492
C	-4.138573	-2.615484	-11.633146
C	-2.632778	-3.880357	-13.617279
C	-4.770375	-3.415919	-12.585080
C	-4.020849	-4.055392	-13.579823

H	-0.911741	-2.978229	-12.692004
H	-4.741506	-2.096188	-10.883940
H	-2.036716	-4.381134	-14.384100
H	-5.855991	-3.540354	-12.554439
H	-4.517682	-4.684702	-14.322244
N	-2.653047	-1.302021	-3.928381
C	-3.679074	-1.464768	-6.160115
C	-3.698373	-1.714769	-4.749310
C	-4.867262	-1.700863	-6.874526
C	-4.819799	-2.372962	-4.174740
H	-4.894661	-1.397154	-7.920531
C	-6.030696	-2.233929	-6.296850
C	-5.944378	-2.622017	-4.931962
H	-4.807846	-2.670061	-3.127890
H	-6.786036	-3.128232	-4.456476
C	-7.293531	-2.366004	-7.053943
C	-7.308615	-2.428505	-8.464528
C	-8.535459	-2.394303	-6.381936
C	-8.509152	-2.502366	-9.168809
C	-9.736580	-2.464183	-7.086653
C	-9.730165	-2.516106	-8.484665
H	-6.369621	-2.441442	-9.020763
H	-8.568755	-2.324477	-5.292925
H	-8.494961	-2.555322	-10.260442
H	-10.683025	-2.468526	-6.540492
H	-10.670101	-2.568684	-9.039292
C	-2.673031	-1.698026	-2.534699
C	-3.429302	-0.987811	-1.597617
C	-1.940703	-2.823212	-2.146441
C	-3.464071	-1.423698	-0.272008
C	-1.975903	-3.246744	-0.818545
C	-2.747730	-2.565088	0.143839
H	-4.006279	-0.115748	-1.913789
H	-1.346286	-3.362334	-2.887382
H	-4.083914	-0.885378	0.447938
H	-1.385661	-4.115783	-0.520928
C	-2.811303	-3.047259	1.547247
C	-2.854832	-2.143386	2.625522
C	-2.828772	-4.426879	1.830437
C	-2.905122	-2.604213	3.942971
C	-2.885259	-4.886771	3.147585
C	-2.920154	-3.977217	4.209216
H	-2.820535	-1.067902	2.433321
H	-2.823823	-5.149262	1.010249
H	-2.925850	-1.887258	4.767529
H	-2.908585	-5.961248	3.347376
H	-2.960870	-4.339094	5.239910

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[2–H]+_os

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N	-2.148029	-7.780693	-9.997780
C	-1.373871	-6.855557	-10.688567
C	-1.795902	-8.317835	-8.748314
C	-3.315511	-8.318815	-10.653918
C	-0.169927	-6.324430	-10.099565
B	0.189836	-6.709042	-8.643036
C	-0.661699	-7.812702	-8.057080
C	-2.575074	-9.348320	-8.206895
C	1.324348	-6.175669	-7.733834
C	-0.338616	-8.399965	-6.799185
C	-2.207066	-9.948287	-6.977872
H	-3.463517	-9.705317	-8.719129
C	-1.099038	-9.464471	-6.273306
N	0.768968	-7.938414	-6.097096
N	-2.958478	-11.012232	-6.478506
H	-0.825907	-9.928233	-5.331264
C	1.579875	-6.866774	-6.508667
C	1.053499	-8.550645	-4.819952
C	-2.893693	-11.333413	-5.083541
C	-3.660073	-11.916234	-7.326733
C	-4.572980	-7.767689	-10.392485
C	-3.180133	-9.398311	-11.533733
C	-5.705755	-8.310843	-11.006338
H	-4.654879	-6.925794	-9.701710
C	-4.314057	-9.933163	-12.149871
H	-2.187979	-9.811435	-11.729423
C	-5.577551	-9.391948	-11.885819
H	-6.689774	-7.887305	-10.789431
H	-4.209180	-10.779286	-12.833201
C	-3.396856	-10.435555	-4.130871
C	-2.329915	-12.548860	-4.671662
C	-3.332226	-10.756241	-2.772762
H	-3.840432	-9.495345	-4.466556
C	-2.269808	-12.864797	-3.312152
H	-1.943696	-13.239690	-5.423904
C	-2.770271	-11.970261	-2.360210
H	-3.734848	-10.059616	-2.033493
H	-1.824498	-13.811006	-2.993778
C	-4.914948	-12.403259	-6.923779
C	-3.099368	-12.374764	-8.532788
C	-5.591643	-13.337367	-7.709748
H	-5.350366	-12.043505	-5.989218
C	-3.793268	-13.292850	-9.323626
H	-2.116581	-12.015717	-8.845034
C	-5.036487	-13.785925	-8.913546
H	-6.560164	-13.719409	-7.376290
H	-3.342270	-13.647383	-10.254405
C	2.655578	-6.466274	-5.675348
C	3.445629	-5.379171	-6.020202
H	2.867135	-7.003912	-4.752966
C	2.132608	-5.047320	-8.010321
C	3.176491	-4.645825	-7.187167
H	4.267827	-5.085665	-5.362491
H	1.916596	-4.449285	-8.894670
H	3.777260	-3.770662	-7.445542
C	0.463406	-8.027167	-3.665210
C	1.909303	-9.653619	-4.747990
C	0.741256	-8.607482	-2.424817
H	-0.205387	-7.167754	-3.750466
C	2.186587	-10.228921	-3.503839
H	2.354105	-10.050001	-5.663326
C	1.606590	-9.704947	-2.343250
H	0.281094	-8.197259	-1.522284
H	2.857929	-11.088745	-3.440512
H	1.833142	-10.155585	-1.373520
H	-2.728708	-12.224841	-1.297996
H	-5.568459	-14.517123	-9.526872
H	-6.462508	-9.819216	-12.364234
C	-0.951632	-5.634856	-12.762594
N	-1.394140	-5.216276	-14.013164
C	-0.657847	-4.369982	-14.862441
C	-2.662543	-5.706343	-14.482401
C	-1.775479	-6.448436	-11.971461
C	0.350471	-5.247619	-12.284804
H	-2.727727	-6.786702	-12.364076
C	0.638593	-5.559061	-10.949803
B	1.319868	-4.536018	-13.255740
C	0.681734	-4.037616	-14.529279
C	-1.246108	-3.898822	-16.041348
C	2.837852	-4.280874	-13.112476
C	1.407035	-3.208651	-15.433715
C	-0.530862	-3.015321	-16.890139

H	-2.249234	-4.203994	-16.323495
C	0.782570	-2.653412	-16.567346
N	2.749237	-2.939838	-15.185094
N	-1.144188	-2.537941	-18.048212
H	1.320489	-1.964340	-17.210153
C	3.475067	-3.467606	-14.100103
C	3.472607	-2.168151	-16.168923
C	-0.387589	-2.015253	-19.140494
C	-2.568525	-2.495815	-18.158264
C	-2.765552	-6.890762	-15.188110
C	-3.855197	-5.004538	-14.237231
C	-3.934122	-7.438029	-15.668597
C	-5.071474	-5.514199	-14.703808
H	-3.809858	-4.064090	-13.682141
C	-5.117959	-6.720400	-15.414466
H	-3.952123	-8.380706	-16.222685
H	-5.993147	-4.961851	-14.506844
C	0.710456	-2.718039	-19.665286
C	-0.762121	-0.791883	-19.717306
C	1.430362	-2.190285	-20.738518
H	1.001079	-3.672312	-19.220934
C	-0.050452	-0.281217	-20.804962
H	-1.615775	-0.247887	-19.308026
C	1.053433	-0.971860	-21.315341
H	2.283795	-2.744632	-21.137404
H	-0.359960	0.667199	-21.251717
C	-3.198793	-3.104213	-19.254956
C	-3.338210	-1.823803	-17.194852
C	-4.587283	-3.037885	-19.386793
H	-2.589754	-3.619446	-20.000603
C	-4.727880	-1.769781	-17.327408
H	-2.837199	-1.344016	-16.351015
C	-5.355085	-2.369682	-18.425867
H	-5.073870	-3.512364	-20.242889
H	-5.322235	-1.239989	-16.578667
C	4.865140	-3.202501	-14.009085
C	5.615784	-3.737295	-12.972054
H	5.360572	-2.586139	-14.756562
C	3.661511	-4.841817	-12.107036
C	5.022002	-4.578496	-12.017974
H	6.683446	-3.509164	-12.915128
H	3.220073	-5.527381	-11.384329
H	5.623316	-5.028542	-11.224707
C	3.931295	-2.794666	-17.333514
C	3.722612	-0.811342	-15.945896
C	4.653640	-2.057894	-18.275111
H	3.714134	-3.853124	-17.494620
C	4.462083	-0.083120	-16.882773
H	3.349601	-0.341182	-15.033247
C	4.926966	-0.704438	-18.047234
H	5.010677	-2.546162	-19.185188
H	4.680065	0.971763	-16.698147
H	5.502055	-0.132599	-18.779411
H	1.615601	-0.564716	-22.159144
H	-6.440299	-2.308811	-18.539671
H	-6.072114	-7.112092	-15.778449
H	1.575941	-5.186652	-10.551386

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C	-2.412822	-1.059828	-9.127562
C	-1.654501	-0.775214	-7.976754
C	-0.350953	-0.212695	-8.183356
C	0.203105	-0.275496	-5.795383
C	-1.042323	-0.867574	-5.469635
C	-1.995827	-0.775505	-10.435880
C	0.096195	0.067653	-9.500840
C	1.164866	-0.015786	-4.799699
C	-1.249185	-1.244016	-4.112097
C	-0.279854	-0.985685	-3.114583
C	0.922947	-0.353417	-3.454155
H	2.119366	0.426235	-5.058776
H	-0.454277	-1.275786	-2.081831
C	-0.710582	-0.195599	-10.587790
H	-3.369340	-1.559661	-8.996059
H	1.080600	0.503479	-9.662988
H	-0.344133	0.069647	-11.580862
B	-2.108586	-1.070543	-6.521370
N	0.500313	0.055003	-7.114319
C	1.772637	0.690654	-7.366780
C	1.862943	2.086207	-7.503581
C	2.965757	-0.008633	-7.388942
C	3.110966	2.701732	-7.615133
C	4.218019	0.549490	-7.473525
C	4.309668	1.960935	-7.578671
H	0.945256	2.680629	-7.491854
H	3.162848	3.789786	-7.692778
H	5.125180	-0.060674	-7.482831
C	5.633999	2.627034	-7.639643
C	6.668494	2.230300	-6.770943
C	5.879845	3.667438	-8.555002
C	7.913975	2.856761	-6.816464
C	7.132105	4.284080	-8.608568
C	8.151426	3.879711	-7.740106
H	6.479737	1.453243	-6.026129
H	5.091865	3.978678	-9.245854
H	8.697261	2.555833	-6.117003
H	7.316403	5.080623	-9.333886
H	9.127898	4.368481	-7.779490
C	-2.861174	-1.035218	-11.607225
C	-2.312546	-1.234592	-12.892335
C	-4.267177	-1.051815	-11.482701
C	-3.132814	-1.419319	-14.005003
C	-5.087236	-1.239128	-12.594519
C	-4.524743	-1.417261	-13.863586
H	-1.228991	-1.262875	-13.026260
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H	-6.173517	-1.228159	-12.472377
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C	-3.476834	-1.564359	-5.977891
C	-3.526856	-2.017867	-4.620642
C	-4.681695	-1.598266	-6.706133
C	-4.715814	-2.610435	-4.123396
H	-4.690304	-1.151373	-7.698213
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C	-5.854110	-2.664531	-4.901984
H	-4.744967	-3.026759	-3.118700
H	-6.741826	-3.147098	-4.489612
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C	-7.116568	-2.101282	-8.412643
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H	-10.465825	-2.074341	-9.075191
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C	-2.712157	-3.534465	0.162744
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C	3.424882	3.152073	-3.529855
H	1.414381	2.415362	-3.290491
C	4.806974	2.899978	-3.414210
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H	3.079984	4.131009	-3.868633
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C	7.983168	4.992264	-3.580791
H	7.292645	3.371117	-2.341781
C	7.682982	5.874068	-4.624393
H	6.207870	6.445286	-6.103120
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H	8.410841	6.627089	-4.936574
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C	2.040115	-0.916111	-1.336040
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H	2.348876	-4.135926	-0.271247
H	2.300240	-3.008908	1.936832
C	2.167664	-3.046137	-2.727169
C	2.959539	-2.634437	-3.814960
C	1.311213	-4.147299	-2.908639
C	2.854006	-3.265951	-5.055853
C	1.205190	-4.781686	-4.149390
C	1.961752	-4.329816	-5.234622
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H	1.863135	-4.811220	-6.210644

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C	-0.170107	3.345693	-7.144173
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C	-0.557448	0.526895	-2.862834
C	-0.482042	-0.534624	-1.928004
C	0.017960	1.781506	-2.539562
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C	0.588555	1.989031	-1.253832
C	0.633635	0.931749	-0.346306
H	0.214159	-1.145352	0.052790
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H	1.088289	1.094921	0.633273
C	-2.000101	-1.000051	-4.357362
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C	-3.389783	-3.435286	-4.543251
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H	-2.346041	-4.044213	-2.775311
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H	-1.018844	-4.952619	1.122909
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C	1.927035	4.414169	-3.403012
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H	-1.957949	0.066153	-9.117705
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C	-4.136245	-3.775208	-7.557570
H	-3.948260	-4.715534	-7.016426
H	-4.860284	-3.989569	-8.359972

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H	-4.034836	-1.050803	-7.974746
C	-6.032531	-3.126039	-6.014706
H	-6.767881	-3.290566	-6.818324
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H	-6.437909	-2.362314	-5.332757
C	2.445087	7.858831	-1.877006
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C	1.514501	8.712119	-0.998134
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C	2.808357	8.668161	-3.143924
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H	3.502792	6.937233	-0.185777
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H	2.635312	-4.907175	1.845629
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H	3.436956	-5.341233	0.317689
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H	2.326417	-7.107451	-1.249936
H	2.191737	-8.237565	0.108850
H	0.738240	-7.790857	-0.823443
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H	-0.366790	-7.173877	1.434284
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1-TS

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C	-2.616655	-1.583262	-9.331126
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C	-2.070993	-1.808492	-10.600152
C	-0.107813	-0.531033	-9.907390
C	0.580716	1.060386	-5.381917
C	-1.493354	-0.628677	-4.471104
C	-0.502528	-0.142647	-3.558978
C	0.483711	0.708923	-4.018574
H	1.094472	1.983884	-5.639138
H	-0.575477	-0.367401	-2.495923
H	1.158102	1.183309	-3.302327
C	-0.786744	-1.278380	-10.856494
H	-3.560538	-2.071375	-9.089691
H	0.893152	-0.173025	-10.141800
H	-0.313266	-1.458696	-11.824199
B	-2.415335	-0.845788	-6.845873
N	0.027996	0.456163	-7.670752
C	1.218567	1.160710	-7.996979
C	1.328384	2.045647	-9.089295
C	2.313796	1.105181	-7.140193
C	2.481790	2.807102	-9.258387
C	3.451828	1.864825	-7.244129
C	3.567329	2.742560	-8.354399
H	0.478066	2.179874	-9.762127
H	2.520480	3.520383	-10.083560
H	4.274317	1.762725	-6.531517
C	4.765353	3.592894	-8.541041
C	5.411837	4.173595	-7.431527
C	5.253716	3.881961	-9.830946
C	6.497192	5.033135	-7.607903
C	6.339858	4.741761	-10.005476
C	6.961566	5.324339	-8.895519
H	5.035624	3.981793	-6.423267
H	4.789518	3.411481	-10.701455
H	6.977119	5.488858	-6.738198
H	6.709273	4.958352	-11.011298
H	7.808892	6.000383	-9.034817
C	-2.791551	-2.608562	-11.617738
C	-2.114042	-3.571324	-12.390501
C	-4.169960	-2.418532	-11.834850
C	-2.794701	-4.323421	-13.350420
C	-4.845328	-3.158842	-12.807506
C	-4.160945	-4.114383	-13.567361
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H	-4.707787	-1.660842	-11.257932
H	-2.255549	-5.075596	-13.931767
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H	-4.692420	-4.696274	-14.324373
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C	-4.941577	-1.522364	-6.876770
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H	-4.996279	-1.180174	-7.910230
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C	-5.975344	-2.471030	-4.931299
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C	-7.432661	-2.201116	-8.414555
C	-8.608046	-2.127105	-6.305327
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H	-8.664309	-2.304747	-10.181840
H	-10.760802	-2.151965	-6.412951
H	-10.809783	-2.263425	-8.910711
C	-2.576908	-1.769494	-2.621674
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C	-1.899502	-2.941304	-2.275985
C	-3.280131	-1.493009	-0.329707
C	-1.911428	-3.382179	-0.952810
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H	-3.799943	-0.129108	-1.931514
H	-1.362045	-3.501393	-3.044472
H	-3.849844	-0.934827	0.415769
H	-1.357136	-4.285155	-0.689422
C	-2.656528	-3.175354	1.445097
C	-2.667653	-2.284132	2.535151
C	-2.693019	-4.557517	1.714282
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C	-2.736888	-5.031394	3.026878
C	-2.742774	-4.134052	4.099308
H	-2.616845	-1.207079	2.356528
H	-2.714606	-5.271824	0.887601
H	-2.705769	-2.050523	4.680289
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2-TS

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B	0.144941	-6.639477	-8.559614
C	-0.667680	-7.786483	-8.007603
C	-2.574126	-9.328845	-8.164081
C	1.280579	-6.110939	-7.651470
C	-0.303838	-8.414854	-6.780537
C	-2.169760	-9.960489	-6.964946
H	-3.473758	-9.676656	-8.662685
C	-1.040044	-9.501486	-6.276430
N	0.817611	-7.962357	-6.088395
N	-2.904440	-11.040772	-6.468135
H	-0.739339	-9.998110	-5.360127
C	1.586787	-6.850110	-6.467612
C	1.136059	-8.619700	-4.844271
C	-2.813300	-11.382784	-5.081204
C	-3.623957	-11.927379	-7.317757
C	-4.624986	-7.610482	-10.253089
C	-3.316579	-9.288351	-11.423467
C	-5.790966	-8.118811	-10.834016
H	-4.660203	-6.766799	-9.560116
C	-4.483811	-9.793416	-12.002157
H	-2.343817	-9.735550	-11.640488
C	-5.721778	-9.210869	-11.707189
H	-6.755412	-7.665137	-10.590639
H	-4.426171	-10.648770	-12.679537
C	-3.237329	-10.472111	-4.101769
C	-2.299358	-12.630149	-4.698954
C	-3.137970	-10.808610	-2.750004
H	-3.642589	-9.506583	-4.412672
C	-2.208771	-12.963478	-3.345440
H	-1.972957	-13.331514	-5.469531
C	-2.625456	-12.053990	-2.367727
H	-3.475562	-10.098873	-1.990873
H	-1.800901	-13.934323	-3.051920
C	-4.871380	-12.421609	-6.900393
C	-3.087111	-12.363705	-8.542697
C	-5.562368	-13.343230	-7.688876
H	-5.289431	-12.077231	-5.952129
C	-3.794439	-13.270152	-9.334779
H	-2.112081	-11.994923	-8.867296
C	-5.029213	-13.772174	-8.909495
H	-6.524799	-13.730764	-7.344140
H	-3.360237	-13.609462	-10.279309
C	2.670922	-6.455074	-5.643457
C	3.413741	-5.323772	-5.951940
H	2.924566	-7.031681	-4.755446
C	2.041569	-4.941415	-7.891278
C	3.089974	-4.542159	-7.072675
H	4.242038	-5.034081	-5.299881
H	1.779259	-4.309366	-8.739840
H	3.652090	-3.632757	-7.297801
C	0.571686	-8.143983	-3.656231
C	1.985676	-9.729866	-4.833923
C	0.865646	-8.779680	-2.447404
H	-0.093182	-7.278134	-3.692595
C	2.278608	-10.362626	-3.621540
H	2.408509	-10.091477	-5.773827
C	1.721557	-9.887492	-2.429254
H	0.423411	-8.406098	-1.520193
H	2.942774	-11.230306	-3.608983
H	1.958359	-10.383590	-1.484538
H	-2.555268	-12.319870	-1.309750
H	-5.571755	-14.494145	-9.524572
H	-6.632748	-9.615325	-12.155901
C	-1.073808	-5.427382	-12.622561
N	-1.538507	-4.930809	-13.854208
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C	-2.788404	-5.324097	-14.424261
C	-1.853670	-6.312707	-11.862835
C	0.237267	-5.063312	-12.157493
H	-2.777478	-6.706221	-12.267353
C	0.546752	-5.418914	-10.836971
B	1.240076	-4.434815	-13.146198
C	0.623788	-3.948237	-14.437239
C	-1.351282	-3.603862	-15.863032
C	2.778005	-4.279842	-13.040970
C	1.388976	-3.222012	-15.397231
C	-0.554451	-2.937033	-16.848774
H	-2.423365	-3.461382	-15.911433
C	0.795957	-2.710990	-16.576132
N	2.739749	-3.031563	-15.179195
N	-1.145454	-2.499148	-18.022240
H	1.391971	-2.134932	-17.274899
C	3.450137	-3.562003	-14.076998
C	3.492906	-2.302240	-16.175427
C	-0.377932	-1.903655	-19.079540
C	-2.525374	-2.762338	-18.324805
C	-2.835644	-5.585641	-15.793889
C	-4.017214	-5.343955	-13.737863
C	-3.976818	-5.839162	-16.516229
C	-5.194029	-5.667400	-14.422439
H	-4.059852	-5.067140	-12.683634
C	-5.183279	-5.928454	-15.797592
H	-3.954334	-5.968194	-17.600965
H	-6.136629	-5.686931	-13.870738
C	0.685111	-2.592168	-19.683849
C	-0.730178	-0.626861	-19.535724
C	1.403110	-1.992092	-20.721235
H	0.953605	-3.588828	-19.326712
C	-0.023065	-0.041014	-20.588683
H	-1.562563	-0.102827	-19.060895
C	1.050066	-0.717572	-21.178333
H	2.233964	-2.530263	-21.184137
H	-0.313594	0.949050	-20.949511
C	-2.836997	-3.695654	-19.323686
C	-3.554996	-2.086226	-17.655884
C	-4.170572	-3.961266	-19.643021
H	-2.025482	-4.203909	-19.848257
C	-4.889305	-2.369004	-17.965387
H	-3.303465	-1.343560	-16.894638
C	-5.199896	-3.305753	-18.957623
H	-4.407913	-4.685743	-20.426337
H	-5.687829	-1.844370	-17.435196
C	4.854924	-3.390648	-14.028998
C	5.592556	-3.931775	-12.984685
H	5.373914	-2.844214	-14.814018
C	3.584170	-4.845702	-12.024433
C	4.962735	-4.679912	-11.979359
H	6.675168	-3.782264	-12.963729
H	3.113971	-5.456693	-11.255602
H	5.548649	-5.133345	-11.176613
C	3.948130	-2.960118	-17.323523
C	3.767941	-0.946837	-15.974287
C	4.688919	-2.253201	-18.274409
H	3.715183	-4.018070	-17.465193
C	4.524487	-0.249316	-16.920460
H	3.397578	-0.453205	-15.073002
C	4.983227	-0.900117	-18.071276

H	5.044399	-2.764930	-19.172098
H	4.760233	0.804760	-16.754121
H	5.571648	-0.351952	-18.810894
H	1.609253	-0.253598	-21.994433
H	-6.242182	-3.521020	-19.206955
H	-6.108134	-6.182605	-16.322329
H	1.494124	-5.066330	-10.442982

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3-TS

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C	-2.511606	-0.583647	-9.027039
C	-1.689239	-0.410067	-7.899373
C	-0.353945	0.055780	-8.130479
C	0.218345	-0.034304	-5.745636
C	-0.973653	-0.731608	-5.446712
C	-2.117041	-0.321830	-10.346854
C	0.101814	0.196480	-9.464688
C	1.141436	0.315310	-4.724411
C	-1.111185	-1.242704	-4.126284
C	-0.122884	-1.019849	-3.140777
C	0.984278	-0.205474	-3.409516
H	1.868752	1.102917	-4.879821
H	-0.256484	-1.409349	-2.137946
C	-0.761180	0.037131	-10.532066
H	-3.506001	-0.987786	-8.866026
H	1.142361	0.428733	-9.676449
H	-0.365379	0.201045	-11.535039
B	-2.084165	-0.851796	-6.462876
N	0.517351	0.319602	-7.057220
C	1.846216	0.791961	-7.277671
C	2.165318	1.905717	-8.078551
C	2.914780	0.203304	-6.606577
C	3.490424	2.318720	-8.212659
C	4.221451	0.608667	-6.659278
C	4.550091	1.677107	-7.534665
H	1.366153	2.465419	-8.569762
H	3.707765	3.189474	-8.833849
H	5.002197	0.088922	-6.099514
C	5.958964	2.086606	-7.732994
C	6.871656	2.064028	-6.660943
C	6.417888	2.496599	-9.000681
C	8.199489	2.446101	-6.849746
C	7.750361	2.867348	-9.190375
C	8.644130	2.845600	-8.114627
H	6.531398	1.779708	-5.663908
H	5.733677	2.493676	-9.852835
H	8.882749	2.449478	-5.998310
H	8.095572	3.173493	-10.181382
H	9.684476	3.146438	-8.262997
C	-3.062699	-0.431443	-11.483360
C	-2.607996	-0.515605	-12.816355
C	-4.458616	-0.423525	-11.270309
C	-3.503170	-0.577724	-13.884344
C	-5.354397	-0.488681	-12.336686
C	-4.881980	-0.562827	-13.651482
H	-1.538826	-0.546293	-13.033176
H	-4.860909	-0.331429	-10.259926
H	-3.118564	-0.641552	-14.905485
H	-6.429338	-0.466224	-12.138254
H	-5.582749	-0.606033	-14.488607
N	-2.235838	-1.975377	-3.798591
C	-3.403502	-1.461832	-5.913950
C	-3.366663	-2.076274	-4.623349
C	-4.640835	-1.476764	-6.587903
C	-4.498459	-2.780467	-4.145346
H	-4.725979	-0.923720	-7.520728
C	-5.790553	-2.115242	-6.105275
C	-5.673466	-2.802279	-4.873962
H	-4.454762	-3.307558	-3.194037
H	-6.521156	-3.369676	-4.484454
C	-7.070202	-2.081541	-6.851806
C	-7.095316	-2.028583	-8.260804
C	-8.302732	-2.098854	-6.168335
C	-8.304936	-1.997468	-8.956209
C	-9.512351	-2.063780	-6.863829
C	-9.519371	-2.014102	-8.261712
H	-6.159265	-2.044844	-8.824149
H	-8.315540	-2.114754	-5.075897
H	-8.300718	-1.972460	-10.049265
H	-10.454339	-2.069855	-6.309647
H	-10.465373	-1.990695	-8.808238
C	-2.237763	-2.639702	-2.514632
C	-2.836157	-2.034884	-1.405500
C	-1.574248	-3.861337	-2.376349
C	-2.762104	-2.655066	-0.158550
C	-1.491825	-4.466502	-1.123311
C	-2.081273	-3.877859	0.013315
H	-3.358385	-1.082956	-1.526011
H	-1.099383	-4.318705	-3.247381
H	-3.255941	-2.185579	0.694192
H	-0.936156	-5.400759	-1.022526
C	-1.991680	-4.530401	1.344953
C	-1.928428	-3.764661	2.525351
C	-1.975921	-5.933818	1.462084
C	-1.861161	-4.380131	3.777225
C	-1.907657	-6.549014	2.713397
C	-1.853021	-5.775424	3.876904
H	-1.910219	-2.673882	2.461706
H	-2.049965	-6.555514	0.566784
H	-1.811386	-3.766708	4.680360
H	-1.909244	-7.640032	2.781120
H	-1.805033	-6.259628	4.855510
N	1.879061	0.122162	-2.411412
C	4.274044	0.619045	-2.626398
C	2.944382	1.056688	-2.635517
C	2.668388	2.404611	-2.907421
C	5.304288	1.505090	-2.941545
H	4.495805	-0.424461	-2.392228
C	3.701766	3.280734	-3.230870
H	1.638086	2.761973	-2.867256
C	5.041784	2.847304	-3.281737
H	6.329230	1.128638	-2.965304
H	3.460429	4.326120	-3.433769
C	6.131710	3.755438	-3.722350
C	5.886045	4.762228	-4.676848
C	7.449024	3.599600	-3.249187
C	6.917671	5.576744	-5.146364
H	4.883054	4.886294	-5.091401
C	8.483345	4.408916	-3.723777
H	7.668423	2.849525	-2.486020
C	8.222908	5.399889	-4.677091
H	6.702316	6.340141	-5.898260
H	9.496462	4.266351	-3.338302
H	9.031972	6.030915	-5.052925
C	1.080807	0.307854	-0.082903
C	1.718038	-0.439637	-1.096463
C	2.182262	-1.736821	-0.842066
C	0.935766	-0.282651	1.183907
C	2.015989	-2.310845	0.420222
H	2.665864	-2.291766	-1.649304
C	1.388274	-1.580783	1.434217
H	0.442338	0.288880	1.974000
H	2.380061	-3.322681	0.614142

H	1.247068	-2.027816	2.421415
C	0.592177	1.693127	-0.340672
C	-0.445833	1.942705	-1.254981
C	1.195072	2.781082	0.311455
C	-0.850938	3.250844	-1.532149
C	0.790963	4.090696	0.033810
C	-0.226480	4.330197	-0.895996
H	-0.936102	1.106095	-1.755838
H	2.004625	2.594415	1.021691
H	-1.659006	3.430118	-2.246370
H	1.280052	4.925504	0.542184
H	-0.542624	5.352434	-1.120888

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4-TS

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B	-0.621310	0.203376	-4.602515
C	-0.506024	1.341990	-5.648713
C	-0.998430	1.261177	-6.966108
C	0.045390	2.597042	-5.235206
C	-1.072781	2.342887	-7.850241
C	-0.127940	3.723873	-6.067519
C	-0.671277	3.592630	-7.339073
H	-1.346983	0.290514	-7.314089
H	0.153799	4.717147	-5.730499
C	0.194173	0.424475	-3.336511
C	0.295768	-0.584952	-2.342539
C	0.890426	1.638299	-3.137052
C	1.081208	-0.365927	-1.161217
C	1.747873	1.813800	-2.000728
C	1.782981	0.811791	-1.010107
H	1.152426	-1.142073	-0.401120
H	2.543613	2.555477	-2.003925
H	2.426058	0.953627	-0.138599
C	-1.474526	-1.089876	-4.608913
C	-2.471317	-1.403566	-5.565596
C	-1.274682	-2.027968	-3.551391
C	-3.225749	-2.578260	-5.551748
C	-2.012738	-3.236582	-3.532046
C	-2.955871	-3.494121	-4.507713
H	-2.665518	-0.669153	-6.341459
H	-1.859209	-3.966331	-2.739639
N	0.731204	2.706007	-4.002459
N	-0.367717	-1.776192	-2.505008
C	-0.081534	-2.857497	-1.583232
C	-0.844512	-3.046275	-0.431363
C	0.967271	-3.731373	-1.882542
C	-0.551998	-4.115299	0.422826
C	1.249656	-4.788356	-1.019842
C	0.495963	-5.013200	0.149357
H	-1.668214	-2.365087	-0.205147
H	1.554562	-3.580129	-2.791041
H	-1.166040	-4.238904	1.314219
H	2.076306	-5.454838	-1.271172
C	1.137885	3.950594	-3.438564
C	0.942064	4.139305	-2.068738
C	1.846672	4.972620	-4.089452
C	1.336301	5.225329	-1.338442
C	2.219764	6.127696	-3.391983
C	1.950054	6.308089	-2.022620
H	2.156203	4.846114	-5.128170
H	1.146121	5.277931	-0.263389
H	2.763291	6.893295	-3.944653
H	-0.779477	4.495838	-7.939809
H	-3.511539	-4.431978	-4.449114
C	-1.619040	2.146282	-9.273379
C	-0.787187	1.062666	-9.997644
H	-0.819020	0.096252	-9.471307
H	-1.182726	0.900007	-11.013067
H	0.268232	1.366031	-10.087205
C	-1.559921	3.440939	-10.102661
H	-1.948739	3.250033	-11.114893
H	-2.176829	4.240582	-9.663481
H	-0.529088	3.815774	-10.207586
C	-3.093942	1.688225	-9.183500
H	-3.506089	1.529573	-10.192978
H	-3.199252	0.744164	-8.628949
H	-3.711705	2.445176	-8.675121
C	-4.302353	-2.916745	-6.593656
C	-3.945428	-4.258223	-7.278818
H	-3.945031	-5.097122	-6.566185
H	-4.687547	-4.491787	-8.058179
H	-2.953345	-4.213626	-7.755873
C	-4.418805	-1.830596	-7.676739
H	-5.201012	-2.104865	-8.400569
H	-4.695332	-0.853405	-7.249253
H	-3.478406	-1.711721	-8.237869
C	-5.671419	-3.064127	-5.886559
H	-6.442702	-3.361124	-6.615582
H	-5.648508	-3.833894	-5.100028
H	-5.984723	-2.116125	-5.419948
C	2.279929	7.598072	-1.256009
C	0.868327	-6.174818	1.087454
C	0.954983	8.258930	-0.804562
H	0.334761	8.537225	-1.671363
H	0.361639	7.589449	-0.162694
H	1.168143	9.173990	-0.229429
C	3.054330	8.598712	-2.131449
H	4.006209	8.176863	-2.492950
H	2.464151	8.924237	-3.002635
H	3.291252	9.497429	-1.542037
C	3.139164	7.257317	-0.016716
H	2.594678	6.632757	0.707942
H	4.058674	6.723786	-0.306511
H	3.431194	8.181262	0.507191
C	2.207507	-5.826249	1.781011
H	2.125413	-4.892115	2.359320
H	2.498327	-6.631382	2.474115
H	3.019978	-5.701924	1.047911
C	1.042502	-7.483235	0.281471
H	1.833718	-7.408034	-0.479173
H	1.325002	-8.304283	0.959179
H	0.107865	-7.766438	-0.229201
C	-0.203740	-6.414762	2.164971
H	-1.184937	-6.637999	1.715044
H	0.081209	-7.276807	2.787234
H	-0.318677	-5.552693	2.840420

Supplementary Table 7. Vibrational frequencies (in cm^{-1}) of the optimized structures

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10.08 12.26 14.25 20.59 24.31 27.63 33.45 42.00
44.15 48.59 62.14 62.90 73.25 79.37 80.69 86.56 89.25
99.55 102.10 121.46 122.85 133.49 140.27 151.79 181.14
190.22 212.93 214.19 217.57 233.82 237.85 258.11
264.00 285.06 323.16 338.40 341.11 346.04 354.52
385.51 404.74 411.88 413.62 419.46 420.73 422.05
423.00 424.42 431.48 432.63 436.71 449.39 457.79
465.29 474.24 483.13 490.37 511.23 522.82 526.11
534.21 536.78 549.37 578.26 583.38 585.41 610.78
628.18 629.70 630.59 632.21 634.12 634.88 643.27
649.51 651.62 657.14 660.87 666.64 679.32 681.33
708.12 712.19 720.76 721.33 722.43 723.98 757.12
758.42 761.52 763.66 767.66 776.12 785.71 787.75
794.49 799.06 799.94 806.38 814.47 846.53 853.05
858.81 859.86 860.41 861.83 862.35 863.82 864.73
866.78 875.33 887.93 926.14 931.53 936.46 939.78
942.23 946.70 950.44 952.94 953.04 962.74 970.84
997.17 997.39 1000.21 1001.91 1002.03 1003.70 1004.03
1004.47 1004.63 1006.11 1006.37 1010.61 1012.32 1012.55
1013.59 1022.97 1023.35 1024.62 1026.27 1028.79 1028.81
1038.62 1041.26 1047.56 1049.01 1063.76 1064.80 1074.25
1080.66 1084.93 1105.77 1106.80 1107.76 1108.29 1118.89
1129.64 1131.29 1133.61 1174.64 1176.79 1177.35 1178.94
1179.07 1192.58 1195.16 1196.48 1202.11 1204.73 1205.87
1207.32 1209.57 1233.60 1240.74 1261.57 1275.75 1276.60
1296.64 1305.86 1306.71 1308.92 1309.03 1311.72 1317.13
1318.57 1319.79 1321.66 1326.17 1329.17 1332.10 1345.54
1347.70 1356.27 1357.37 1359.32 1360.89 1361.92 1362.23
1366.13 1383.62 1385.84 1433.65 1437.44 1439.26 1450.38
1474.29 1475.62 1478.28 1478.99 1479.33 1488.49 1510.96
1517.14 1520.18 1520.67 1533.93 1542.96 1554.09 1555.07
1590.79 1594.30 1612.24 1613.29 1622.92 1628.16 1630.58
1635.53 1635.73 1637.82 1654.79 1658.31 1658.37 1659.66
1660.65 1663.49 1668.46 1669.66 3162.11 3162.77 3165.83
3166.58 3167.92 3168.96 3173.18 3173.34 3173.74 3174.84
3175.01 3180.41 3180.99 3181.66 3182.36 3183.19 3183.87
3184.26 3184.58 3185.70 3188.21 3189.01 3190.06 3193.78
3194.52 3195.41 3195.77 3198.59 3199.14 3200.92 3201.50
3210.16 3218.39 3220.21 3220.80 3228.00 3231.14

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9.95 11.65 14.20 20.09 24.08 28.28 33.26 36.76 45.89
47.61 61.01 70.37 74.98 79.01 79.65 85.76 88.00 96.81
102.84 118.70 124.35 134.70 141.44 151.08 160.71
188.39 208.65 211.27 214.91 232.43 236.10 258.19
262.46 285.69 320.17 330.20 338.69 347.92 352.40
384.93 402.89 410.06 412.76 416.84 419.94 421.16
421.31 425.51 430.29 432.80 435.49 449.30 464.43
473.55 476.92 481.26 484.72 508.39 516.73 524.61
530.06 539.28 548.01 577.05 583.51 590.79 609.06
627.34 629.10 630.55 630.78 632.56 634.30 640.58
648.62 649.97 656.73 659.75 666.98 668.44 681.42
708.24 711.56 717.18 720.87 721.90 724.49 754.87
757.53 760.47 763.08 766.98 770.57 784.07 787.27
794.73 797.23 800.59 806.05 812.73 841.61 850.99
857.60 858.93 860.29 860.56 861.91 863.32 864.39
870.44 875.27 889.93 925.68 934.82 936.28 941.44
943.30 946.69 950.84 951.67 958.05 964.92 982.29
998.72 999.97 1001.44 1001.54 1003.39 1004.34 1005.55
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3239.77 3244.83 3246.30 3248.52 3258.75

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1250.60 1255.98 1257.91 1265.42 1292.60 1302.59 1311.43
1326.53 1333.60 1337.40 1338.73 1356.96 1366.77 1372.55
1383.96 1390.84 1398.75 1402.76 1413.23 1455.42 1473.47
1483.56 1486.23 1486.58 1498.45 1511.32 1515.14 1521.15
1527.94 1534.79 1539.84 1618.96 1624.82 1628.53 1628.65
1631.45 1639.68 1653.49 1657.06 1658.82 1660.75 1677.95
1683.75 3167.23 3167.30 3168.08 3169.53 3173.20 3175.07
3176.55 3177.80 3179.02 3182.49 3188.79 3191.29 3191.76
3192.41 3193.75 3195.64 3196.28 3196.69 3197.54 3201.88
3203.58 3203.90 3204.32 3209.24

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4.65 14.04 28.90 32.62 42.28 49.79 70.75 91.76 105.69
108.77 115.46 144.15 145.74 151.49 168.80 204.81
242.91 248.16 263.23 282.03 295.51 300.98 306.49
342.09 358.20 386.42 417.55 421.61 439.05 442.40
443.98 454.31 463.85 470.17 477.72 494.37 531.09
535.35 560.11 586.92 589.63 592.22 596.99 608.48
626.52 628.57 630.38 642.00 654.00 665.49 677.78
699.48 703.83 720.94 731.75 753.73 759.19 761.56
765.69 778.16 782.28 784.62 787.91 808.88 814.74
828.21 846.50 863.76 864.78 879.79 885.60 888.23
891.99 914.53 919.17 945.83 950.35 955.88 965.16
966.30 968.77 969.35 975.77 984.70 1001.76 1005.56
1006.00 1006.62 1008.88 1011.91 1018.95 1029.64 1031.52
1042.53 1044.58 1048.67 1051.85 1077.37 1095.64 1107.90
1118.02 1127.68 1140.30 1150.81 1168.34 1171.41 1176.40
1179.38 1185.22 1190.60 1206.82 1244.93 1252.26 1256.16
1260.76 1266.36 1294.78 1300.23 1307.47 1331.03 1333.89
1337.35 1339.73 1361.21 1369.94 1386.45 1391.52 1392.01
1401.61 1409.35 1447.17 1473.66 1474.28 1482.88 1486.02
1489.16 1502.82 1511.62 1521.46 1527.43 1532.46 1534.33
1554.46 1621.52 1627.04 1628.59 1630.76 1632.38 1652.82
1653.55 1657.89 1660.07 1677.95 1683.64 3167.60 3168.05
3168.37 3169.10 3174.71 3175.34 3176.74 3176.81 3182.06
3185.66 3186.57 3189.71 3190.80 3191.55 3192.01 3195.62
3197.36 3197.73 3197.96 3202.79 3203.95 3204.58 3210.18

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345.15 355.58 365.06 398.28 415.72 426.70 439.81
443.21 444.57 463.02 465.31 469.67 477.83 492.00
534.52 535.02 562.22 571.40 587.98 589.67 592.36
606.87 608.04 628.18 629.25 635.13 650.05 659.36
677.48 701.09 704.24 731.85 746.80 753.69 758.64
761.70 764.36 769.83 780.43 783.74 794.63 808.01
814.52 821.45 841.97 845.10 879.70 885.74 891.86
900.03 917.76 923.07 927.49 946.23 950.10 951.30
954.21 964.76 965.09 968.83 969.89 973.81 979.07
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1381.63 1389.00 1391.52 1396.82 1400.55 1411.92 1413.94
1449.21 1472.36 1474.96 1485.58 1486.22 1493.38 1511.48
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1677.94 1683.41 2946.30 2968.76 3167.43 3167.95 3168.12
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3201.54 3202.66 3204.33 3208.04 3208.46 3209.45
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763.81 770.90 782.79 784.42 790.98 792.04 801.24
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1010.00 1013.80 1018.04 1024.42 1025.29 1025.34 1026.49
1027.13 1035.41 1044.62 1047.13 1049.66 1052.01 1073.58
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1315.75 1320.22 1328.96 1333.70 1355.79 1360.02 1362.07
1368.63 1380.45 1399.40 1403.29 1415.98 1453.53 1466.25
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1676.08 3168.62 3176.65 3183.20 3185.49 3188.68 3189.15
3189.44 3192.75 3192.97 3195.01 3195.76 3196.80 3200.76
3202.02 3205.32 3207.40 3208.08 3209.14 3210.44 3211.37
3213.65 3218.08 3219.84 3224.98
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322.38 360.28 377.61 410.82 420.61 423.31 435.69
443.87 450.45 461.44 482.61 495.99 502.97 532.14
536.48 543.67 572.62 579.43 591.98 604.55 615.61
622.34 628.09 632.07 651.95 659.62 667.82 676.43
687.85 707.88 722.61 730.64 749.07 754.10 763.32
767.27 776.83 781.85 786.99 788.67 810.77 812.27
825.91 833.19 841.82 864.42 867.59 884.40 898.78
926.63 935.21 938.69 939.25 947.64 956.87 960.60
973.23 979.94 985.04 998.93 1005.66 1009.98 1014.19
1014.63 1020.24 1024.92 1027.77 1030.43 1034.37 1038.22
1040.95 1046.52 1054.35 1072.93 1079.65 1101.87 1108.84
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1481.01 1486.75 1502.80 1515.31 1518.04 1523.88 1537.44
1548.98 1575.32 1605.81 1622.94 1628.20 1630.35 1637.47
1640.62 1655.28 1657.96 1664.69 1670.09 1722.77 2891.20
3170.99 3175.48 3182.00 3185.07 3188.18 3189.48 3190.02
3191.41 3193.53 3197.72 3198.72 3201.39 3201.64 3201.73
3202.98 3203.38 3205.67 3213.58 3215.64 3216.57 3225.19
3228.27
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312.52 321.83 343.21 360.81 390.25 420.67 423.80
429.62 440.57 445.32 456.99 465.24 472.14 474.94
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610.60 611.91 630.07 632.30 639.78 658.10 663.46
676.62 683.41 699.40 721.95 727.82 730.12 753.22
761.03 778.11 781.02 782.62 787.71 789.61 806.89
823.77 826.52 828.43 839.85 848.06 863.94 889.32
897.11 905.52 914.33 919.97 933.44 937.33 955.32
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1004.19 1004.53 1010.67 1014.56 1020.24 1023.20 1027.18
1029.67 1032.77 1033.39 1035.93 1045.40 1047.31 1049.69
1073.76 1108.83 1117.08 1121.00 1131.21 1150.72 1165.67
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1206.86 1242.71 1249.47 1258.02 1268.12 1294.98 1309.11
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1629.24 1631.84 1640.01 1645.56 1649.38 1658.78 1660.73
1665.87 1678.23 1708.14 2985.17 3001.58 3166.78 3172.76
3174.56 3183.33 3185.19 3186.12 3187.90 3188.95 3189.19
3190.46 3190.97 3192.07 3195.68 3197.97 3198.14 3199.71
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[1–H]+_os
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44.49 47.11 51.03 62.08 74.05 79.15 81.35 86.82 90.34
98.55 108.75 123.11 125.29 134.78 136.84 153.66 179.77
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644.55 650.46 651.65 658.63 662.96 673.53 689.53
701.00 705.38 709.68 716.62 721.26 721.96 733.51
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788.12 797.65 801.78 803.54 811.85 848.05 851.35
854.81 857.96 859.38 860.18 863.76 864.16 865.80
871.90 893.13 916.29 921.74 924.49 938.42 939.84
940.93 947.47 954.11 955.37 957.86 959.82 965.97
995.49 995.94 1000.91 1004.21 1005.33 1006.29 1006.56
1007.56 1008.87 1010.67 1011.02 1012.64 1012.85 1014.66
1018.26 1022.03 1033.79 1034.78 1035.23 1035.52 1035.93
1038.97 1045.68 1047.67 1061.90 1064.53 1067.10 1075.64
1082.82 1109.17 1109.40 1109.71 1114.12 1116.92 1131.52
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1194.43 1198.81 1201.16 1204.99 1205.63 1208.56 1210.76
1227.71 1234.03 1242.73 1250.30 1266.17 1273.51 1291.44
1294.32 1304.15 1307.85 1308.69 1309.95 1313.26 1315.97
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1356.60 1361.29 1362.55 1364.11 1367.17 1376.57 1387.85
1392.72 1422.92 1428.27 1437.97 1446.49 1461.30 1473.40
1477.66 1479.44 1480.42 1488.81 1492.38 1506.56 1510.22

1518.36 1530.35 1532.44 1535.35 1548.62 1557.76 1565.08
1569.11 1585.11 1591.49 1613.55 1622.89 1623.09 1629.34
1633.45 1636.11 1646.98 1649.51 1654.06 1655.87 1656.92
1658.24 1660.88 3171.52 3172.11 3172.24 3175.99 3176.14
3177.03 3177.44 3178.14 3181.01 3183.68 3183.80 3185.36
3185.98 3187.47 3188.94 3191.60 3192.23 3192.34 3192.84
3194.05 3197.23 3199.56 3200.38 3201.23 3201.98 3202.78
3202.93 3203.16 3203.93 3206.30 3209.92 3220.82 3229.24
3231.07 3233.64 3242.31
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8.02 8.34 13.22 14.26 16.65 17.80 18.53 22.61 24.44
30.04 32.23 35.12 39.70 43.67 44.33 47.20 48.81 52.02
53.31 55.99 56.69 59.27 60.85 62.53 64.67 68.78 71.47
82.68 87.79 94.65 98.89 104.23 115.29 122.43 142.05
164.33 173.27 185.90 189.19 193.81 199.42 207.40
212.26 215.07 223.51 230.76 235.52 241.02 245.57
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368.13 388.66 405.15 415.38 423.92 424.36 424.99
425.51 426.24 427.02 427.63 429.35 430.74 434.57
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536.59 537.63 540.06 544.87 552.37 563.49 564.26
567.48 611.46 618.53 622.50 624.16 625.63 627.21
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635.04 635.40 641.00 643.62 651.11 658.91 660.78
664.84 668.86 671.58 674.08 678.40 696.83 700.61
704.92 719.88 721.69 721.86 722.47 722.53 725.18
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792.51 795.03 806.14 806.92 809.80 816.83 821.15
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863.71 865.25 876.47 878.29 882.81 885.68 888.32
889.80 893.38 894.61 898.87 902.54 907.33 922.15
926.70 932.02 934.40 939.25 942.23 948.01 949.73
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1015.57 1016.86 1017.18 1017.47 1017.99 1026.28 1027.03
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1600.56 1605.24 1606.86 1615.96 1619.57 1633.05 1633.40
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1659.99 3172.09 3172.72 3174.55 3174.61 3174.68 3176.94
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3204.12 3204.75 3219.83 3223.23 3229.75 3231.83 3250.77
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32.70 35.24 42.89 43.22 44.51 50.45 51.00 59.49 62.70
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1012.92 1013.41 1014.34 1014.87 1017.98 1023.46 1024.35
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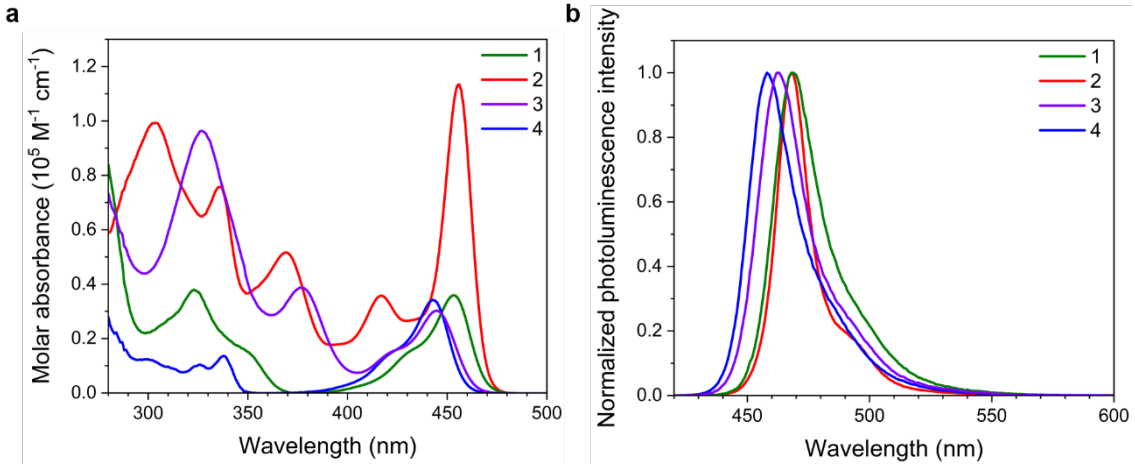
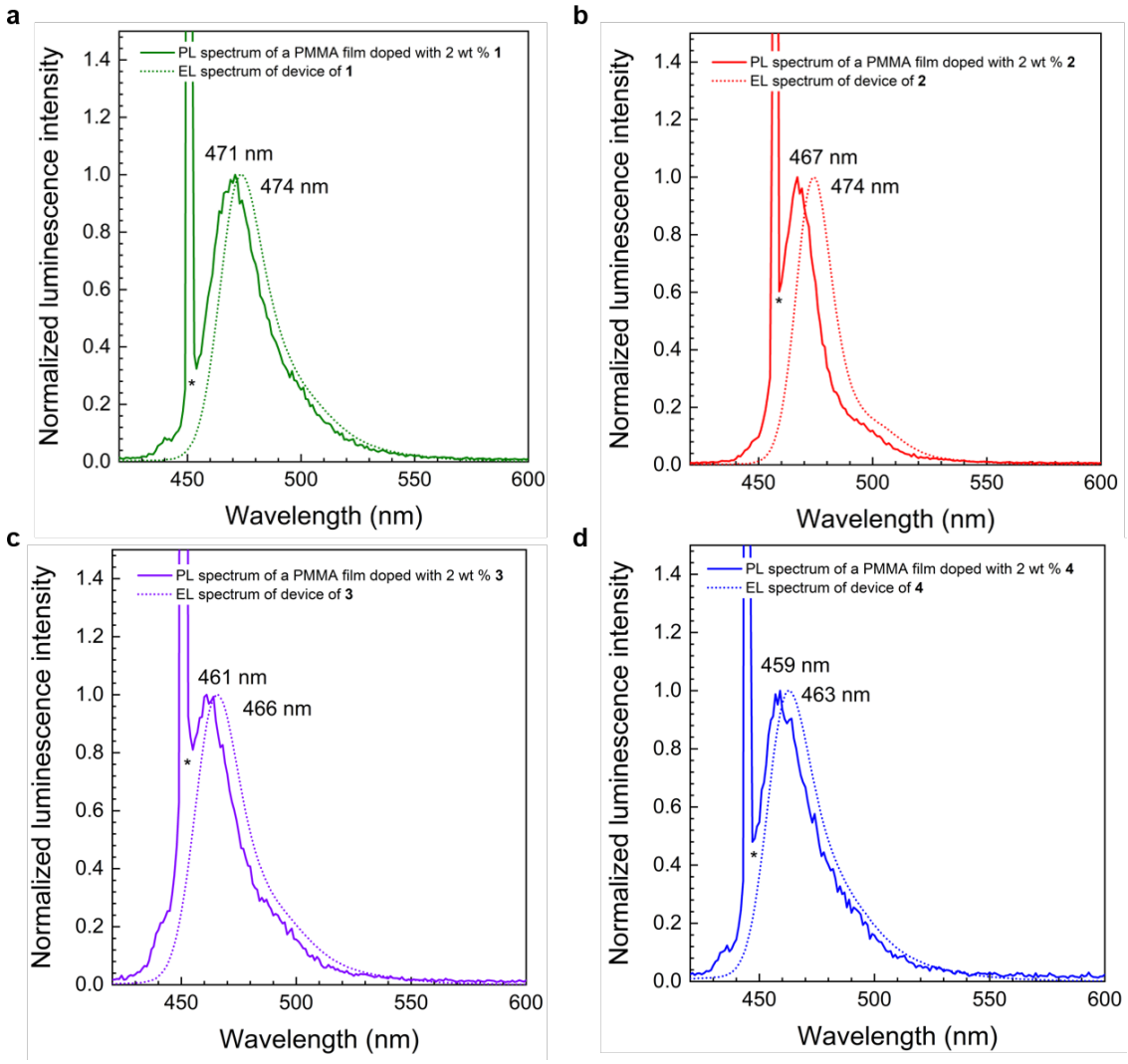
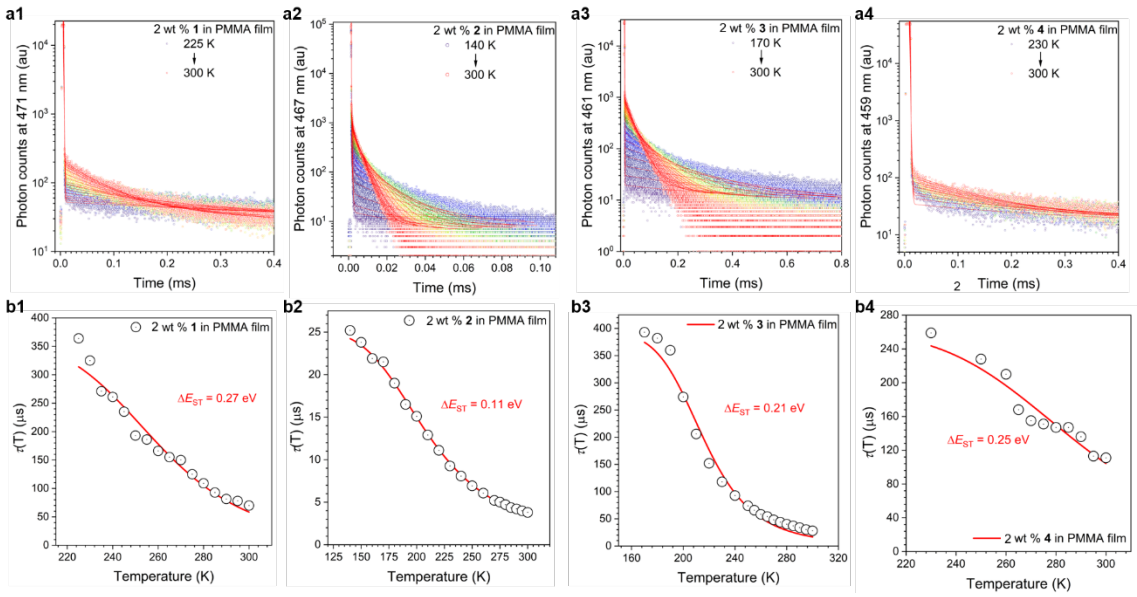


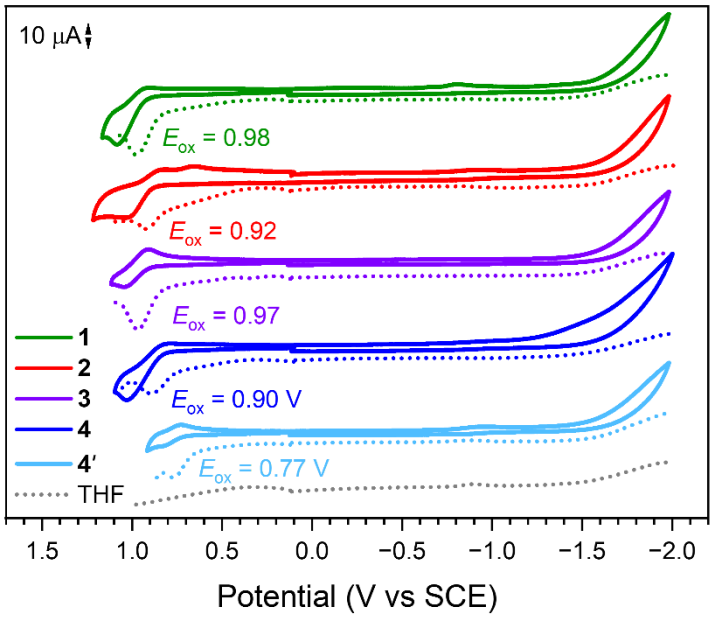
Supplementary Fig. 1 Steady-state photophysical measurements. a,**b**, UV–Vis absorption (**a**) and normalized photoluminescence (**b**) spectra of Ar-saturated THF containing 10 μM dopant. λ_{ex} = 450 nm (**1**, **2** and **4**) and 443 nm (**3**).



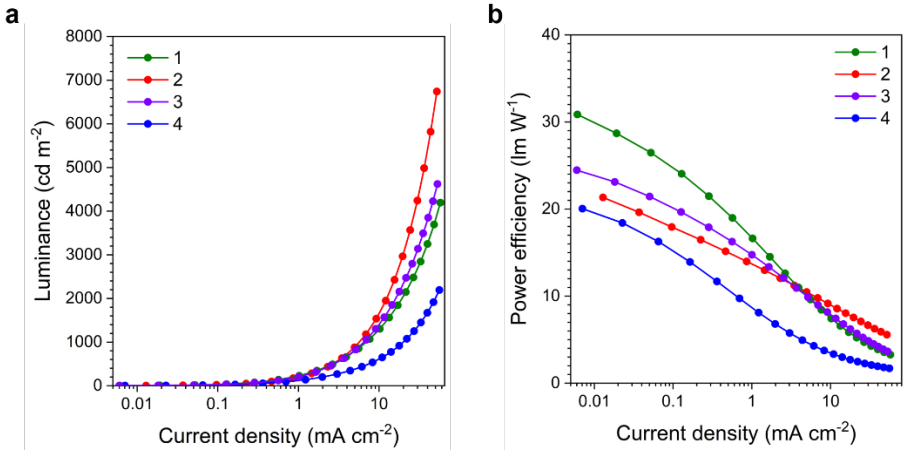
Supplementary Fig. 2 Steady-state photoluminescence spectra. a–d, Normalized photoluminescence spectra of PMMA thick films doped with 2 wt % **1** (**a**), 2 wt % **2** (**b**), 2 wt % **3** (**c**), and 2 wt % **4** (**d**). λ_{ex} = 450 nm (**1** and **3**), 456 nm (**2**), and 444 nm (**3**). The signals marked with an asterisk (*) are due to the excitation beam. Dotted curves are normalized electroluminescence spectra.



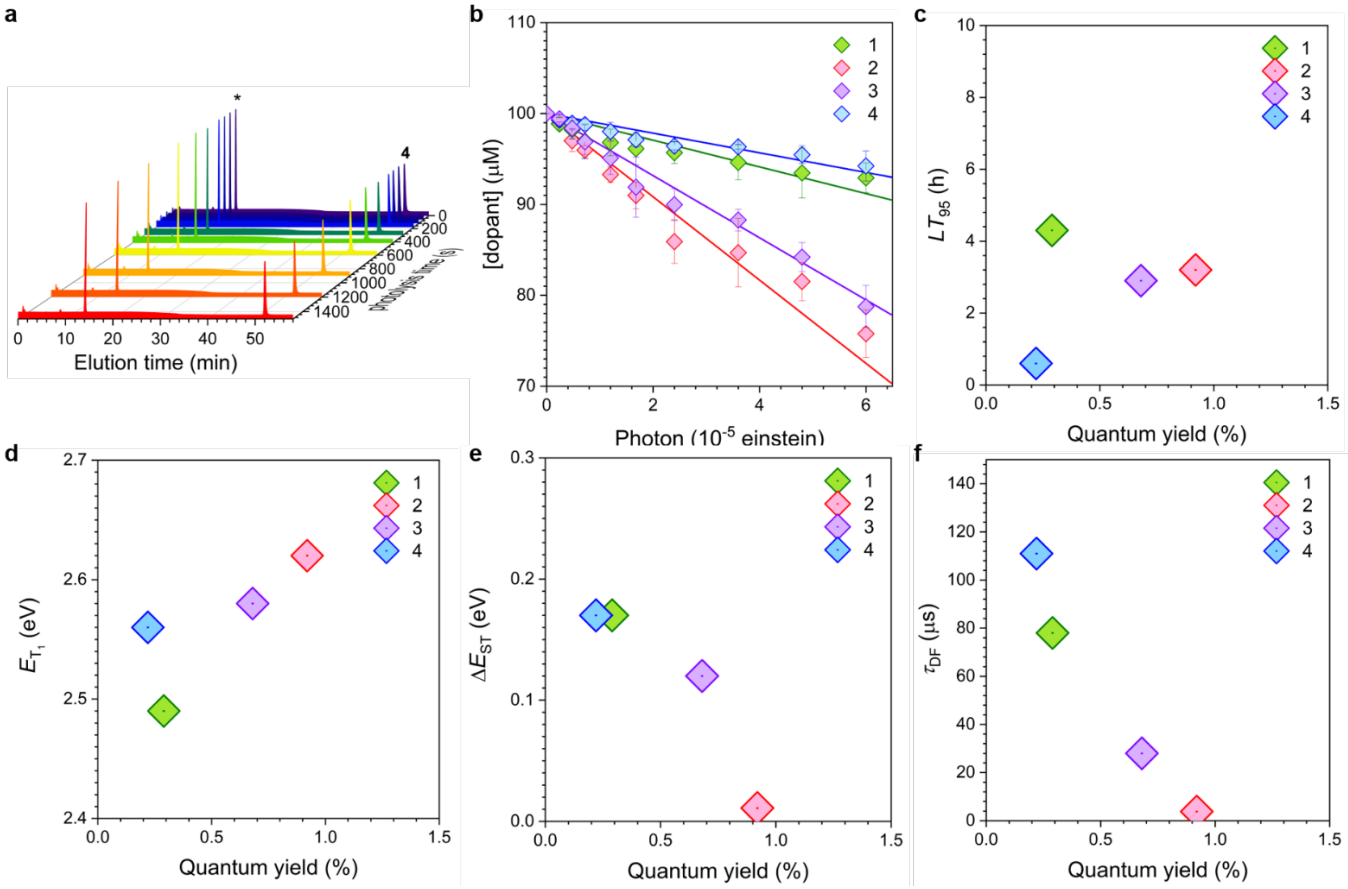
Supplementary Fig. 3 Variable-temperature photoluminescence decay traces. a, Variable-temperature photoluminescence decay traces of PMMA films doped with 2 wt % **1** (**a1**), 2 wt % **2** (**a2**), 2 wt % **3** (**a3**), and 2 wt % **4** (**a4**) recorded after pulsed laser photoexcitation at a wavelength of 377 nm. Red curves are nonlinear least-squares fits of the data points to a biexponential decay model. **b**, Photoluminescence lifetime ($\tau(T)$) as a function of temperature. The red curves are nonlinear least-squares fits of the data points to the equation, $\tau(T) = [3 + \exp(-\Delta E_{ST}/k_B T)] / [(3/\tau_{T1}) + (1/\tau_{S1})\cdot\exp(-\Delta E_{ST}/k_B T)]$ where ΔE_{ST} is the energy difference between the singlet and the triplet excited states, k_B is the Boltzmann constant, T is the absolute temperature, τ_{T1} is the lifetime of the triplet state, and τ_{S1} is the lifetime of the singlet excited state.



Supplementary Fig. 4 Electrochemical potentials. Cyclic (CV, solid lines) and differential pulse voltammograms (DPV, dotted lines) for Ar-saturated THF containing 1.0 mM dopant and 0.10 M tetrabutylammonium hexafluorophosphate. A glassy carbon disc and a Pt wire for the working and counter electrodes, respectively; a $Ag/AgNO_3$ pseudo reference electrode; scan rate = 0.1 V s^{-1} (CV) and 4 mV s^{-1} (DPV). The grey dotted lines are the DPV signals of the blank solution of Ar-saturated THF containing 0.10 M tetrabutylammonium hexafluorophosphate only.

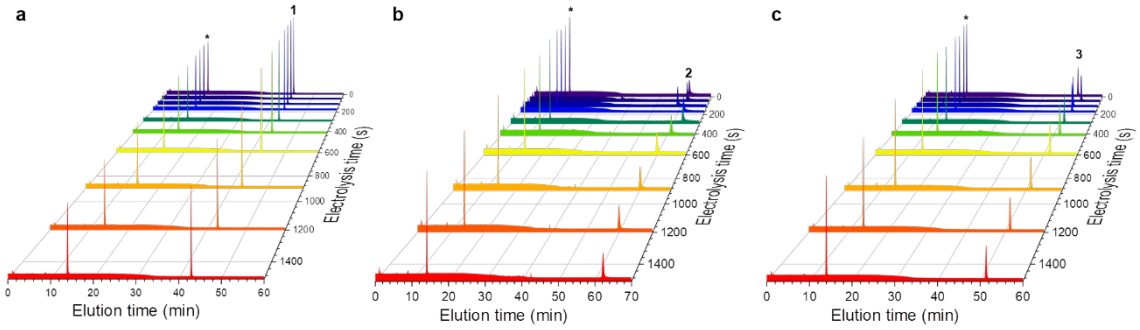


Supplementary Fig. 5 Electroluminescence performances. a, Luminance as functions of current density. **b**, Power efficiency as functions of current density.

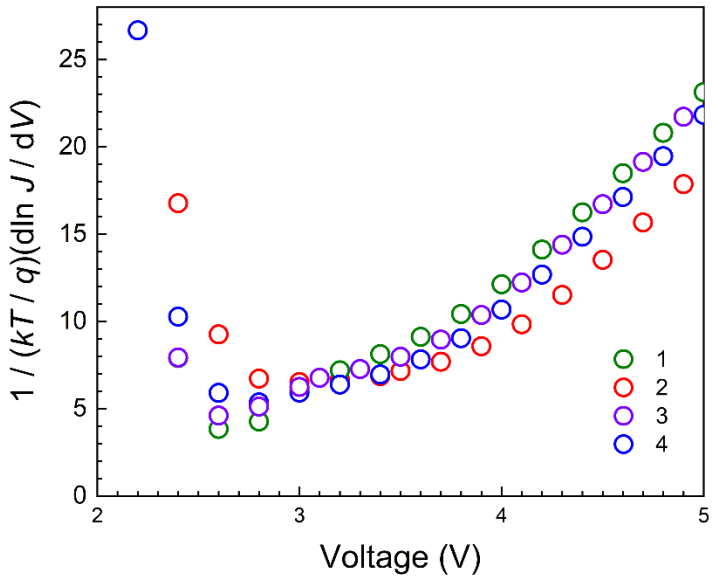


Supplementary Fig. 6 Excitonic degradation. a, Liquid chromatograms of 100 μM **4** (THF) recorded during continuous photolysis under photoillumination with a monochromatic light of a wavelength of 450 nm. The peak marked with an asterisk (*) is a benzophenone internal standard. **b**, Decay in the concentration of the residual MR-TADF dopants during the continuous photolysis. The concentration values were

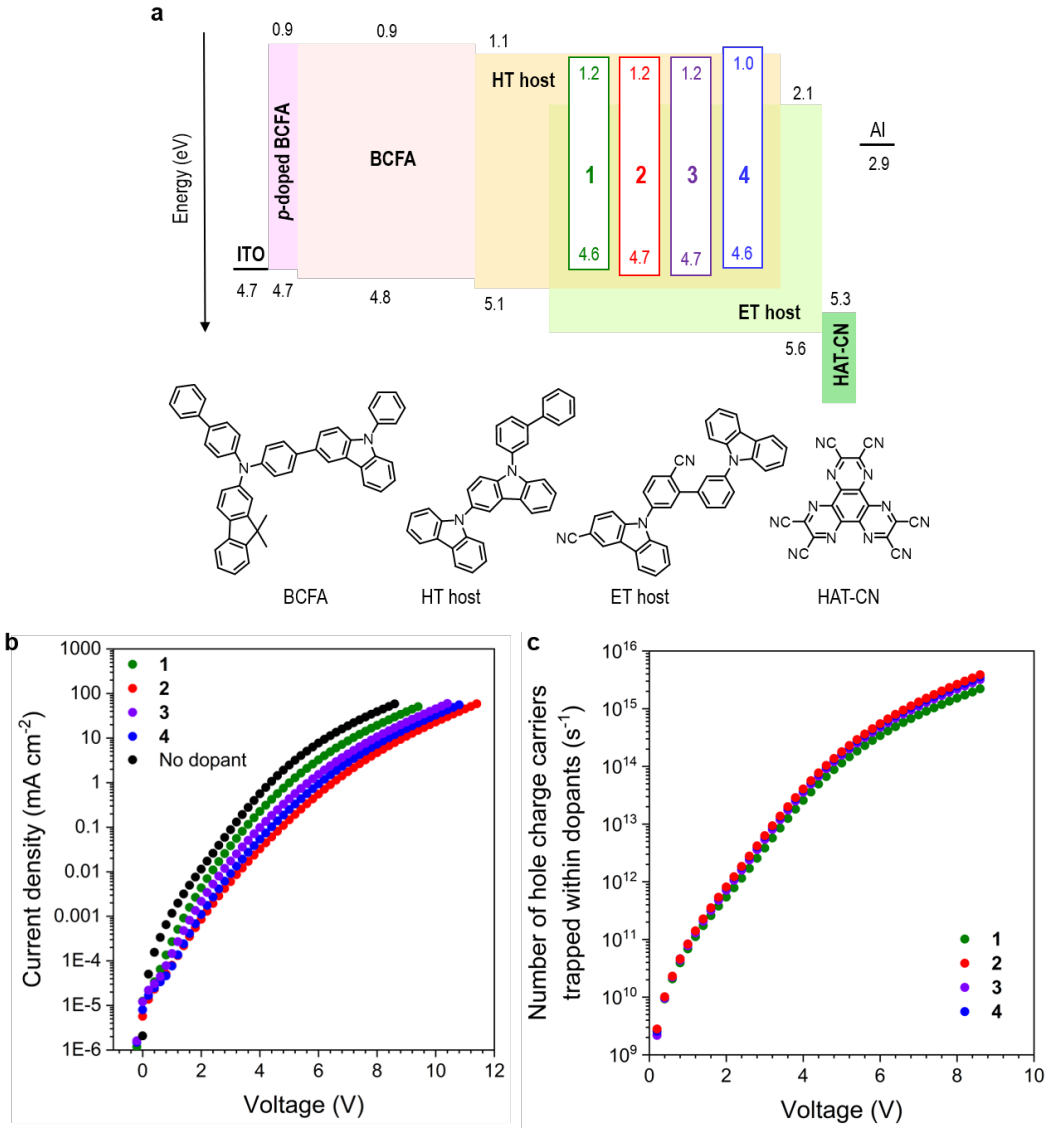
corrected by the different absorptivity of incident photons (4.0×10^{-8} einstein s^{-1}). The standard deviations were obtained from three independent measurements. The solid lines are linear fits of the data. **c**, A correlation between LT_{95} and the quantum yield for excitonic degradation of the dopants. **d**, A correlation between the triplet excited-state energy (E_{T1}) and the quantum yield for excitonic degradation of the dopants. **e**, A correlation between the energy difference between the singlet and the triplet excited states (ΔE_{ST}) and the quantum yield for excitonic degradation of the dopants. **f**, A correlation between the lifetime of delayed fluorescence (τ_{DF}) and the quantum yield for excitonic degradation of the dopants.



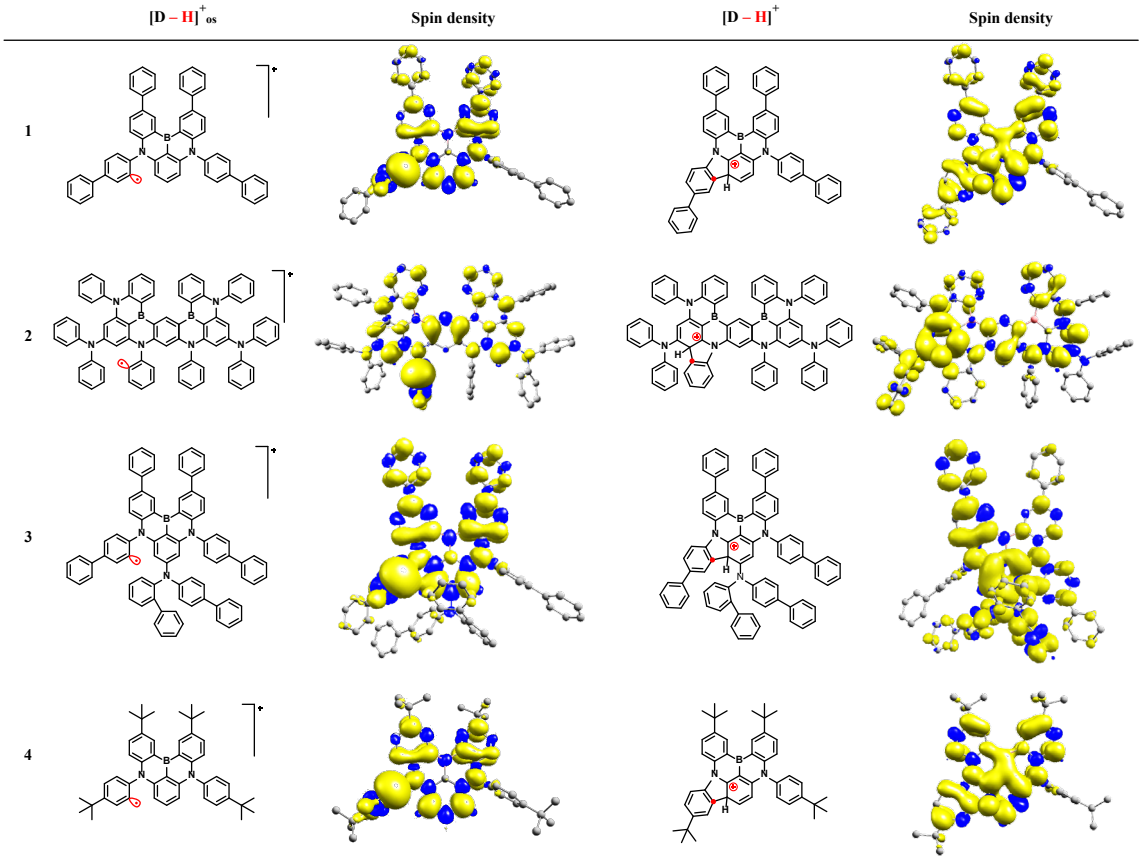
Supplementary Fig. 7 Oxidative degradation. a–c, Liquid chromatograms of 100 μM **1** (**a**), 100 μM **2** (**b**), and 100 μM **3** (**c**) (Ar-saturated THF containing a 0.10 M tetrabutylammonium hexafluorophosphate supporting electrolyte) recorded during oxidative bulk electrolysis at anodic potentials of 1.04 V for **1** and **3** and 1.01 V for **2** vs SCE. A Pt mesh and a Pt coil were used for the working and the counter electrodes, respectively. A $Ag/AgNO_3$ pseudo reference electrode was used. The peak marked with an asterisk (*) is a benzophenone internal standard.



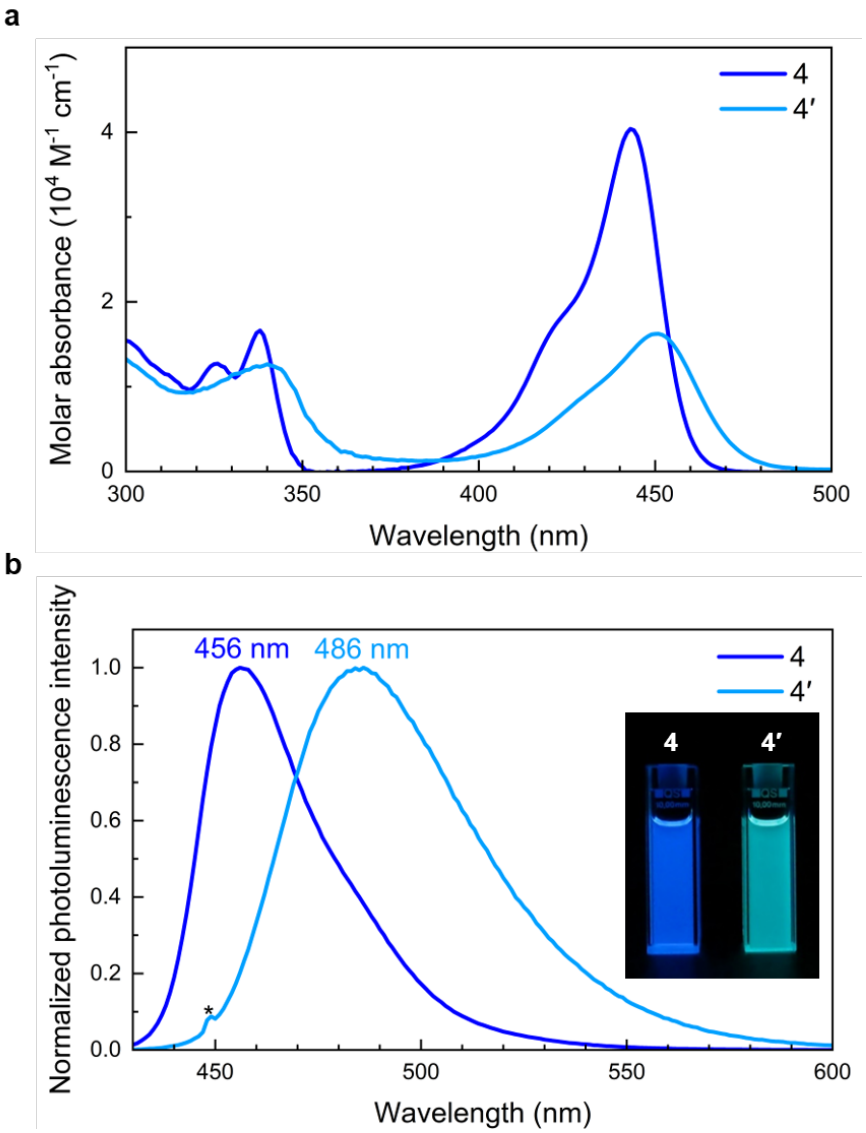
Supplementary Fig. 8 Ideality factor. Plots of $[(k_BT/q)\cdot(\partial \ln J/\partial V)]^{-1}$ as a function of voltage (V) for devices of **1–4**, where k_B is the Boltzmann constant, T is the absolute temperature, q is the elementary charge, and J is the current density.



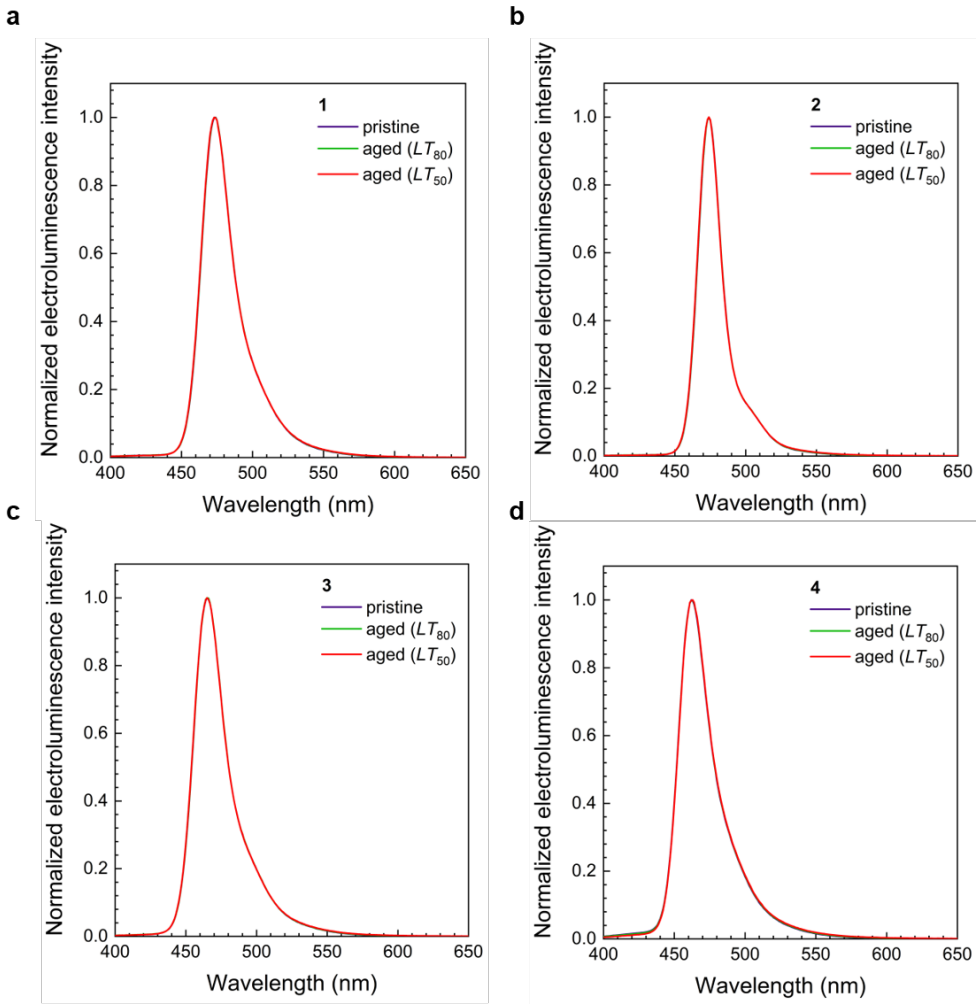
Supplementary Fig. 9 Charge carrier trapping within dopants. a, Schematic of the configuration of the hole-only devices (HODs) tested, including the energy levels and chemical structures of their component materials. The 2 wt % dopants were doped into a 1:1 mixture (wt/wt) of the HT host and the ET host. **b,** Plots of current density of HODs as functions of applied voltage, recorded in the absence and presence of dopants. **c**, The corresponding number of trapped charge carriers per unit time as functions of applied voltage. The number of trapped charge carriers per unit time (η_{trap}) is calculated with an equation $\eta_{trap} = [(J_0 - J) \times A] / q$ (s^{-1}), where J_0 and J are current densities in the absence and presence, respectively, of dopants, A is the active area of the device (0.1225 cm^2), and q is the elementary charge (1.60×10^{-19} C).



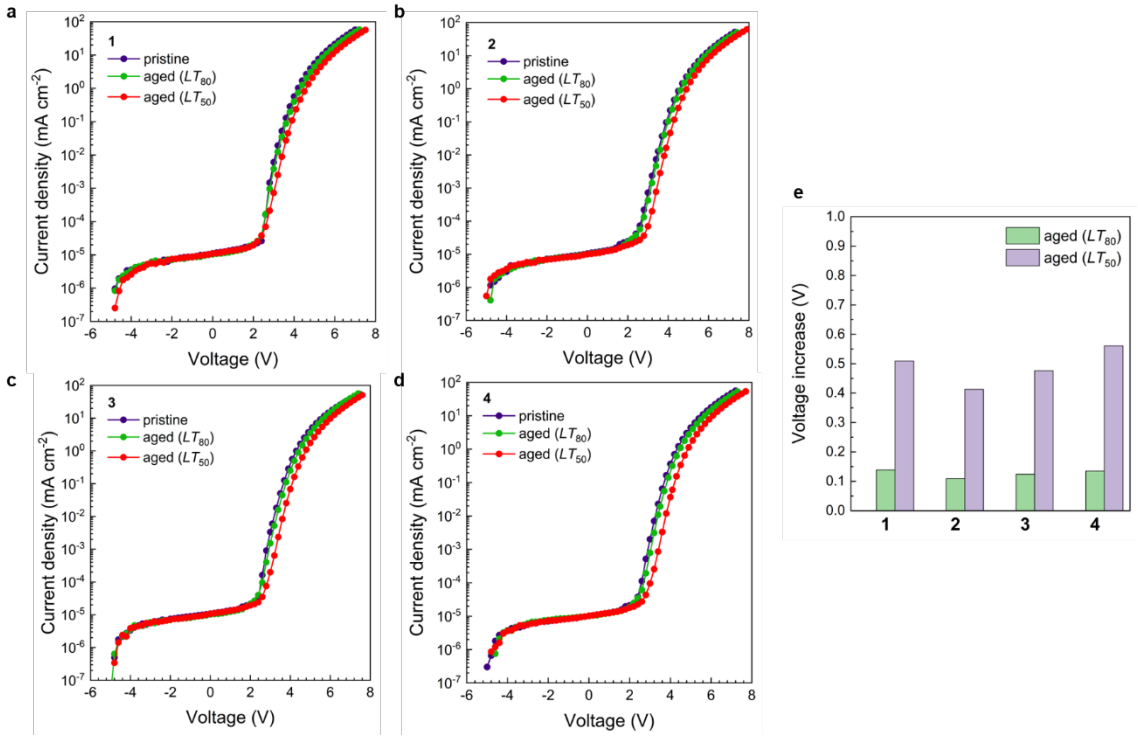
Supplementary Fig. 10 Calculated spin densities of the open-shell intermediate $[D - H]^{+}_{os}$ and cyclized intermediate $[D - H]^{+}$ of dopants 1–4. The spin densities (alpha – beta electron density) were visualized with the isodensity value of 0.005 au.



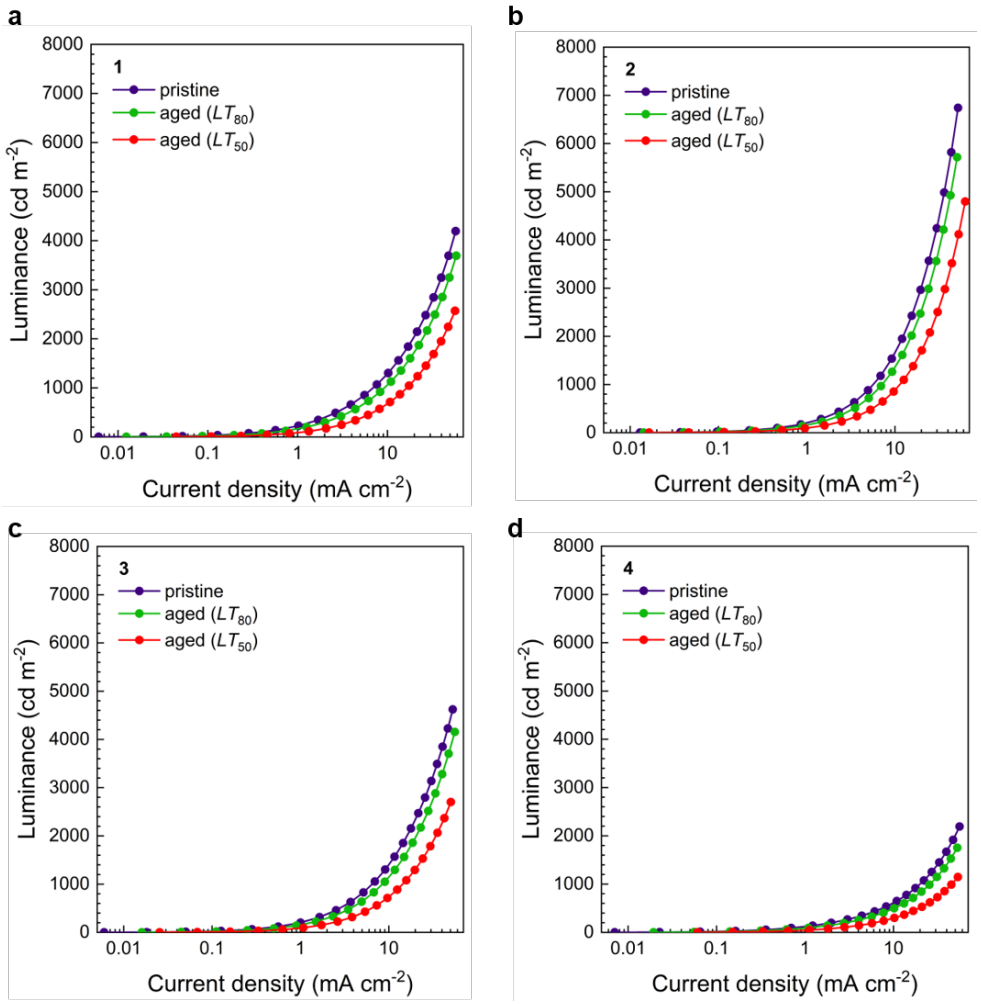
Supplementary Fig. 11 Electronic transition spectrum of the cyclization byproduct. a,b, UV–Vis absorption (**a**) and normalized photoluminescence (**b**) spectra Ar-saturated THF of 10 μM **4** (blue) and 10 μM cyclization byproduct of **4** (**4′**, sky blue). The peak marked with an asterisk is the excitation beam. The numbers are peak wavelengths. The inset photo in **b** shows the photoluminescence emission visualized under photoexcitation at 365 nm.



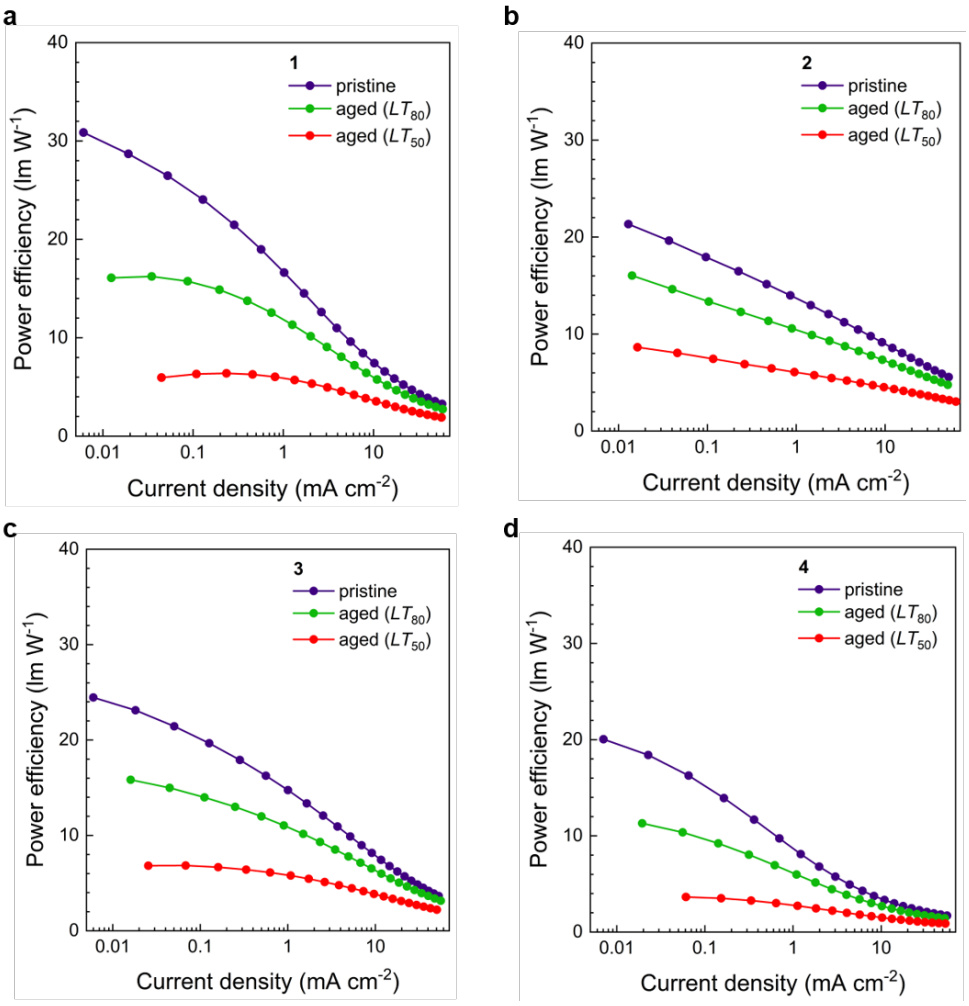
Supplementary Fig. 12 Electroluminescence spectra. a–d, Normalized electroluminescence spectra of the devices of **1** (**a**), **2** (**b**), **3** (**c**), and **4** (**d**) before (pristine) and after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}.



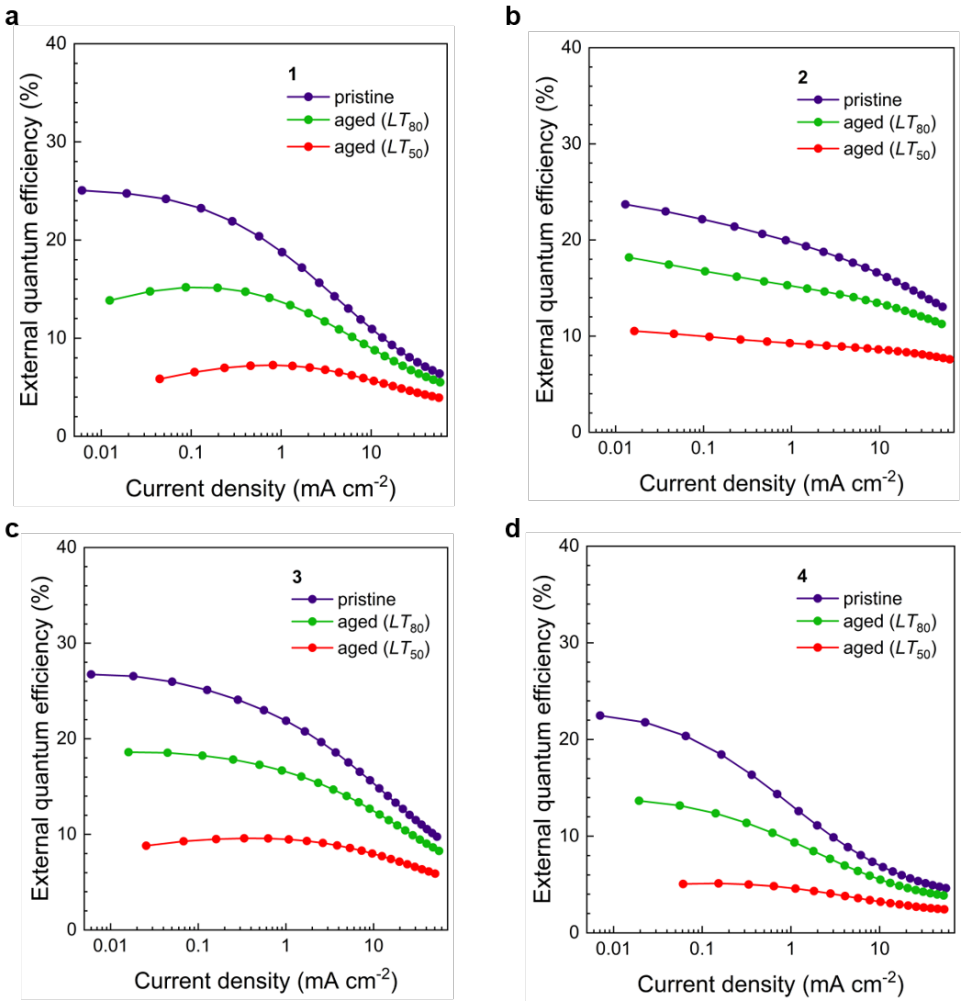
Supplementary Fig. 13 Increased operational voltage. a–d, Current density as a function of applied voltage of the devices of **1** (**a**), **2** (**b**), **3** (**c**), and **4** (**d**) before (pristine) and after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}. **e**, Increase in the operation voltage after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}.



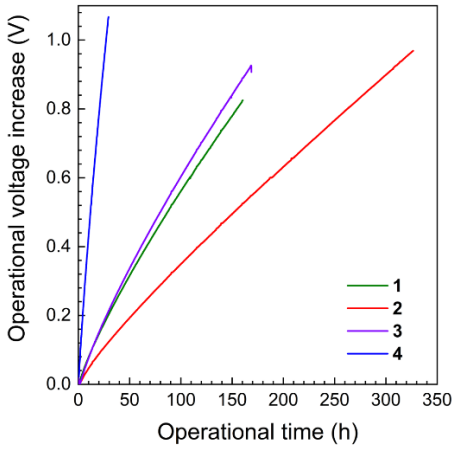
Supplementary Fig. 14 Luminance changes. a–d, Luminance as a function of current density of the devices of **1** (**a**), **2** (**b**), **3** (**c**), and **4** (**d**) before (pristine) and after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}.



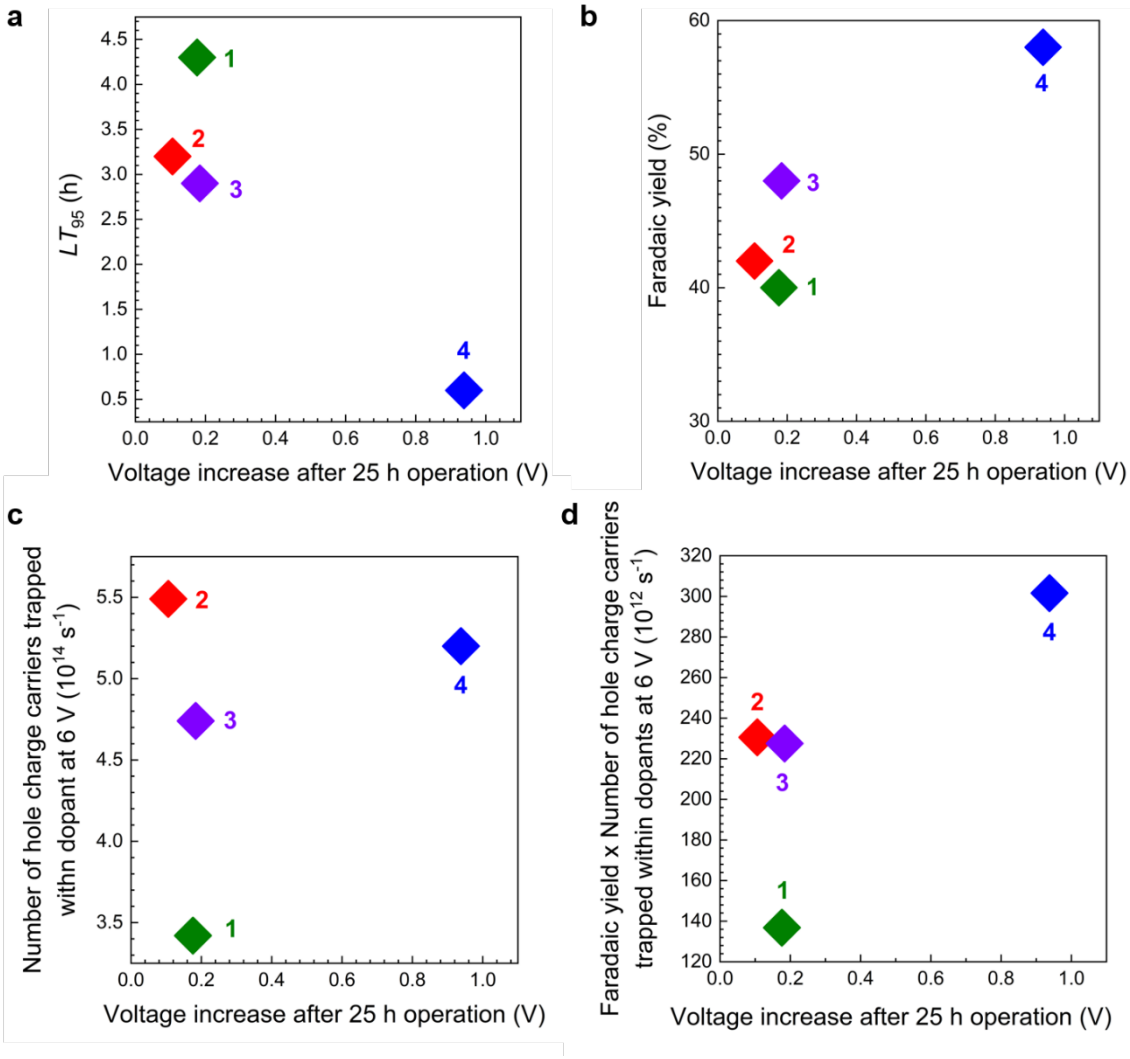
Supplementary Fig. 15 Power efficiency changes. a–d, Power efficiency as a function of current density of the devices of **1** (**a**), **2** (**b**), **3** (**c**), and **4** (**d**) before (pristine) and after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}.



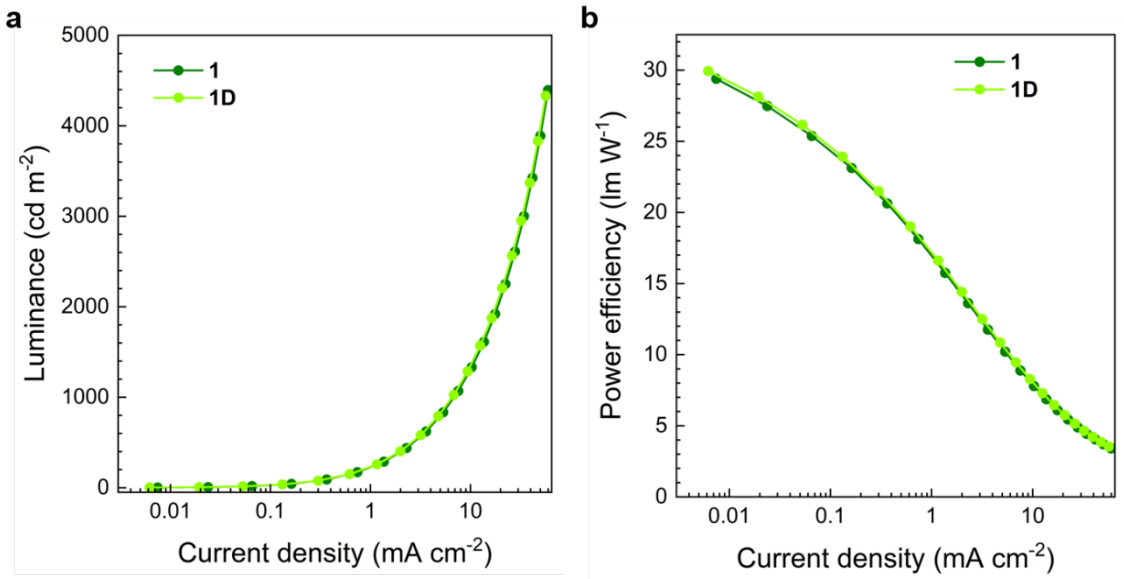
Supplementary Fig. 16 External quantum efficiency changes. a–d, External quantum efficiency as a function of current density of the devices of **1** (**a**), **2** (**b**), **3** (**c**), and **4** (**d**) before (pristine) and after LT_{80} and LT_{50} operation at an initial luminance of 1000 cd m^{-2}.



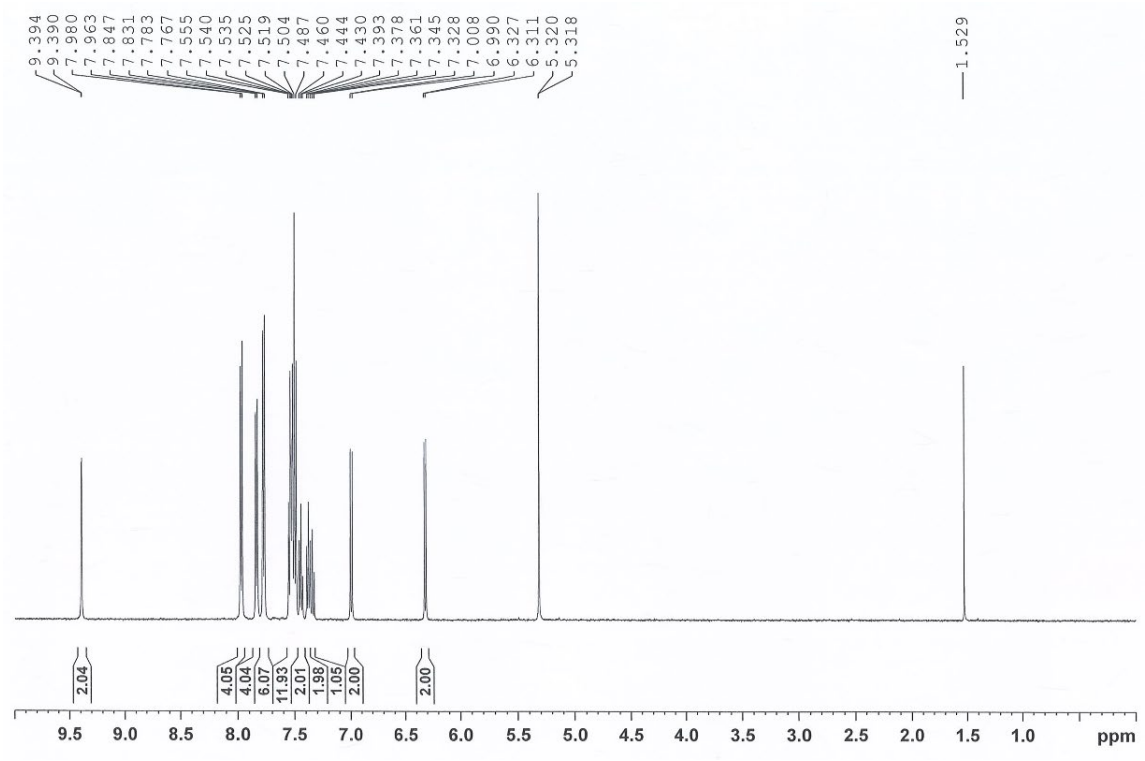
Supplementary Fig. 17 Increased operational voltage. Increase in the operational voltage as functions of operation time driven at constant current density at an initial luminance of 1000 cd m^{-2}.



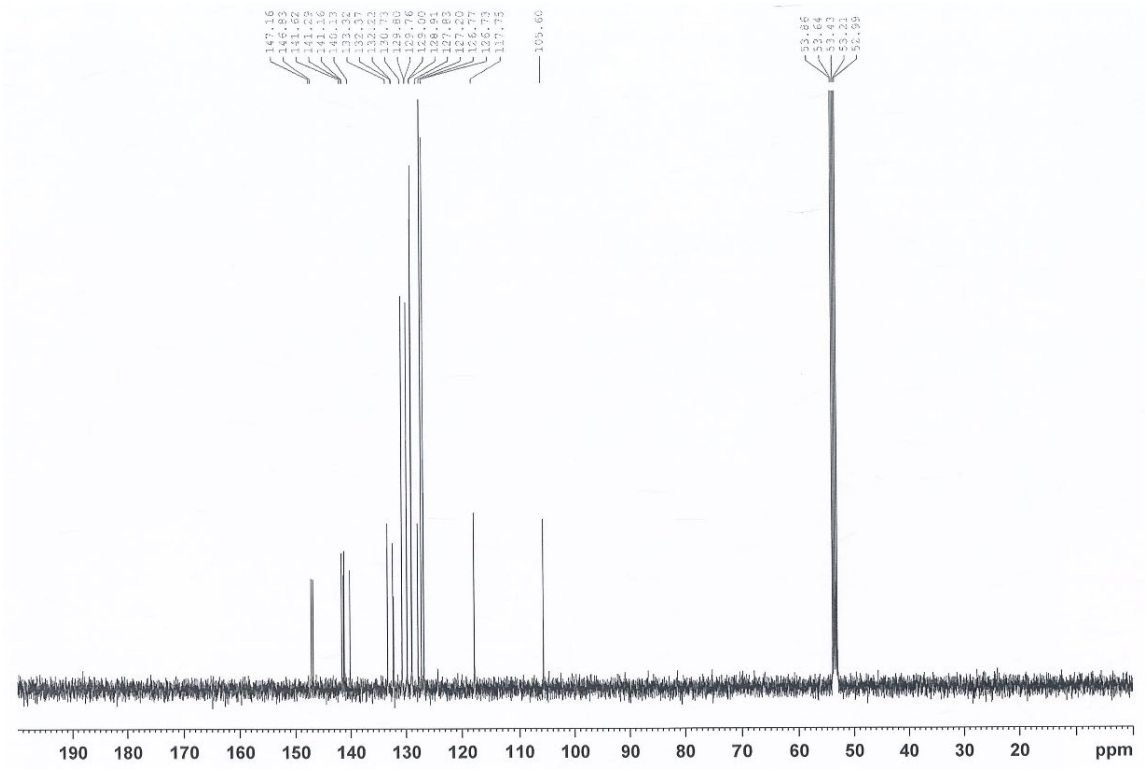
Supplementary Fig. 18 Correlations of stability parameters with increased operational voltage. a–d, LT_{95} (**a**), Faradaic yield (**b**), the number of hole charge carriers trapped within dopants at 6 V (**c**), and a product of Faradaic yield × the number of hole charge carriers trapped within dopants at 6 V (**d**) as functions of the voltage increase after 25 h of operation at constant current densities of an initial luminance of 1000 cd m^{-2}.



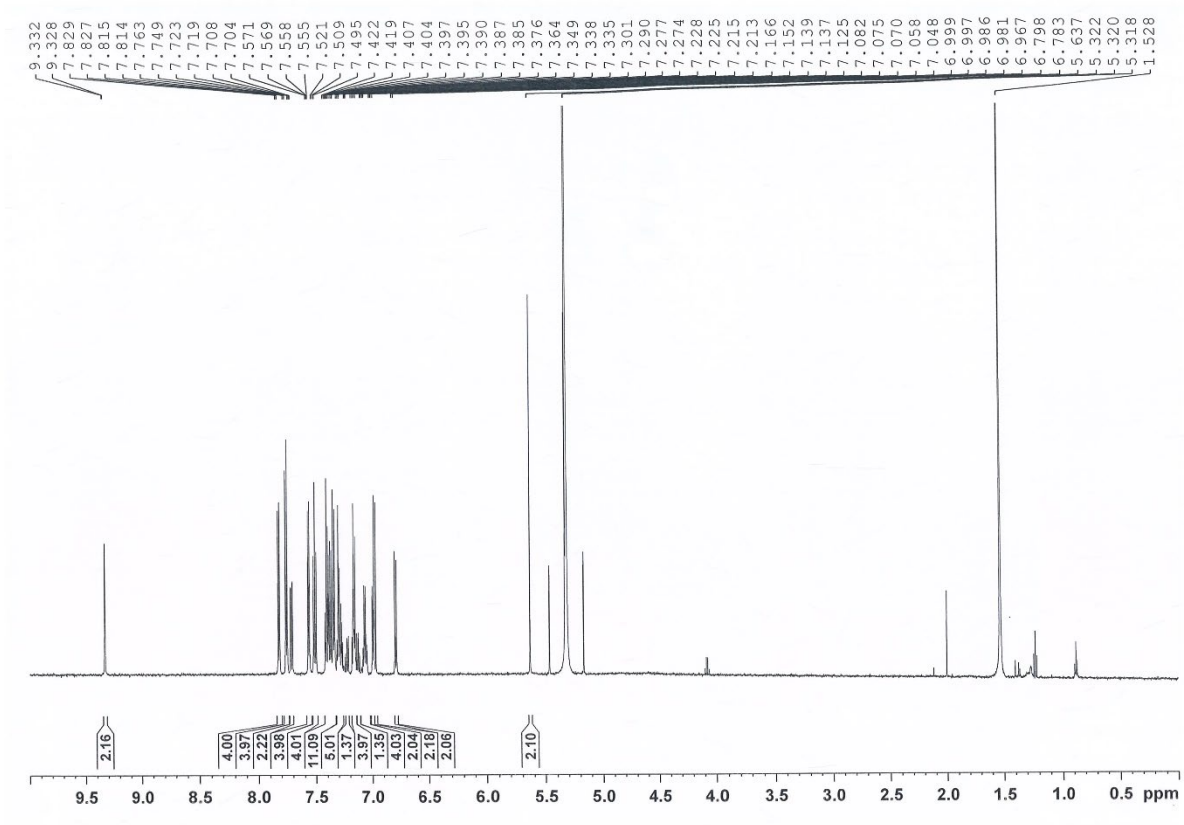
Supplementary Fig. 19 Electroluminescence performances. a,b, Luminance (**a**) and power efficiency (**b**) as a function of current density of devices of **1** and **1D**.



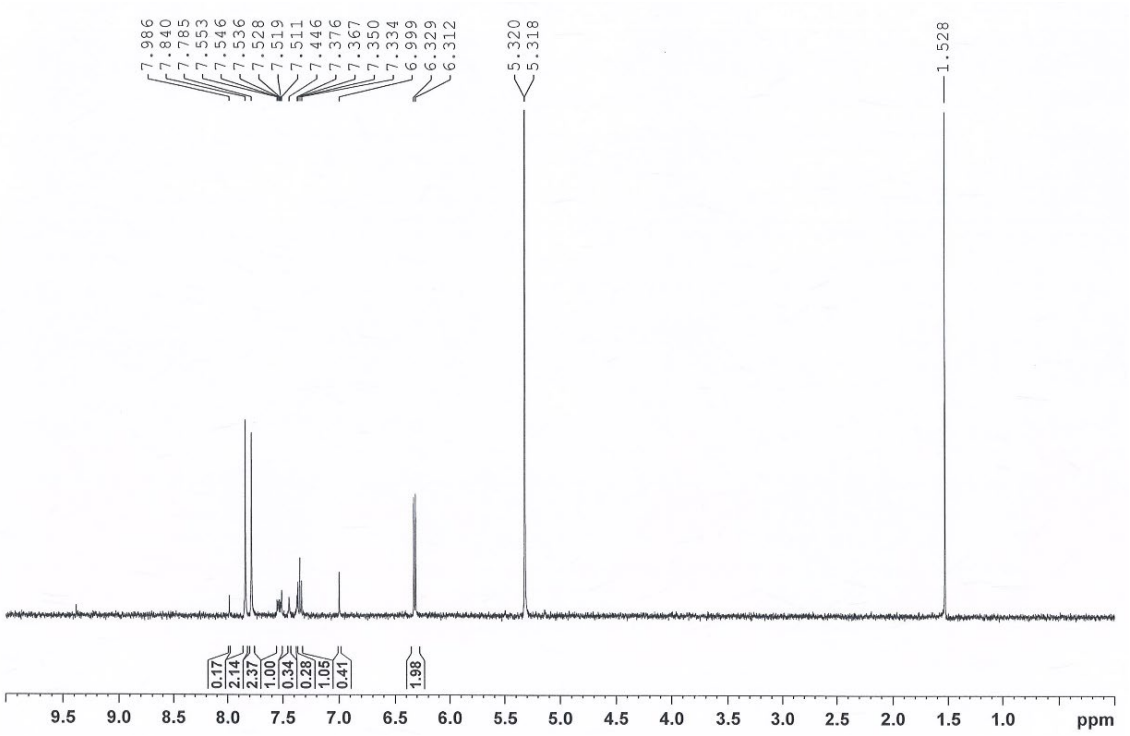
Supplementary Fig. 20 ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **1**.



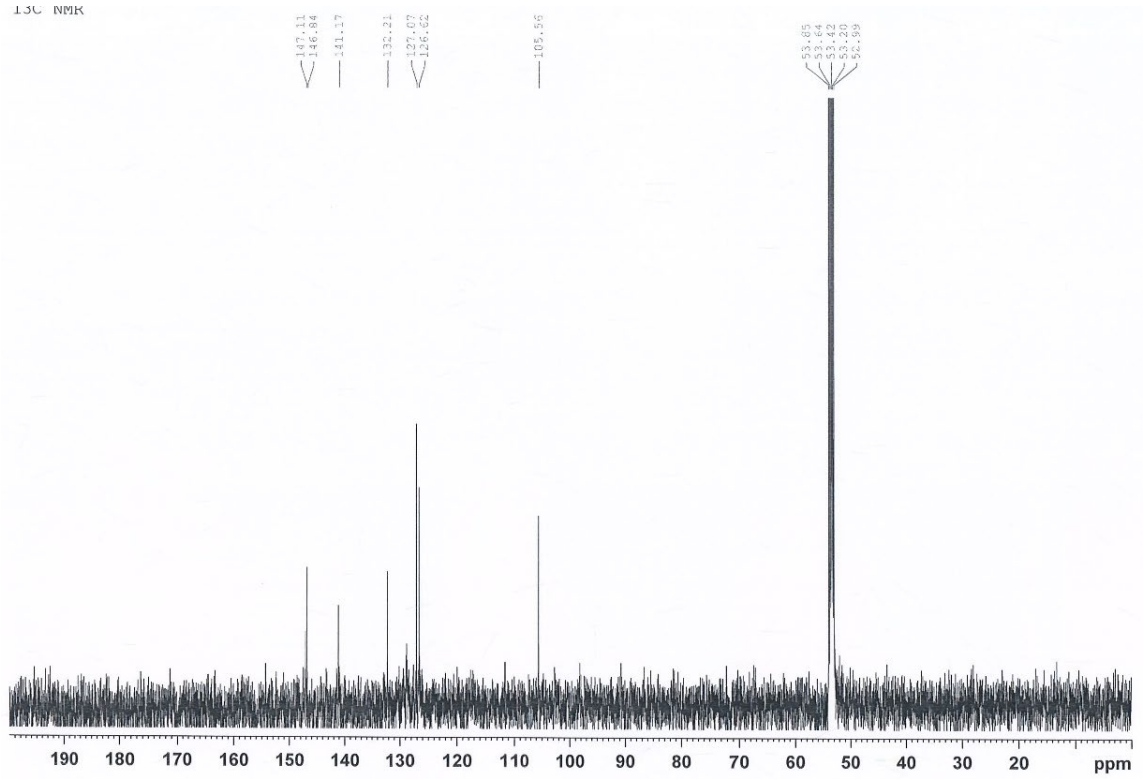
Supplementary Fig. 21 $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2) spectrum of **1**.



Supplementary Fig. 22 ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **3**.



Supplementary Fig. 23 ^{1}H NMR (500 MHz, CD_2Cl_2) spectrum of **1D**.



Supplementary Fig. 24 $^{13}C\{^{1}H\}$ NMR (125 MHz, CD_2Cl_2) spectrum of **1D**.