Supporting Information

Vibronic Transitions Determined Narrowband Emission for Multi-Resonant Thermally Activated Delayed Fluorescence Emitters

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Computational details:

Geometry optimization and frequency computation in ground states were performed by DFT method and for excited state TDDFT method was applied. For multi-resonance TADF molecules whose electronic transition is very local a hybrid functional B3LYP[1-3] was applied with D3 correction[4], and the basis set was cc-PVDZ[5-8] supported by Gaussian 16 (C.01 version)[9]. For D-A type TADF molecules whose electronic transition is in a broad range a range-separated functional CAM-B3LYP[10] was applied with D3 correction[4]. The geometries for the optimization in ground state was generated by conformer searching supported by the Crest module in XTB program[11-15]. For the computation of a spin-orbital coupling matrix DKH method was used, and the basis set was DKH-def2-TZVP[16-17] a special version for DKH method (the auxiliary basis is SARC/J[16-17]) provided by ORCA (5.0.2 version)[18-19] based on a converged geometry in triplet state optimized using open-shell unrestricted DFT method. The vibrationally resolved electronic spectra and the vibronic intensities containing HT effect were computed by MOMAP program[20-31]. The FHWM in the calculation of spectra was set as 1200 cm^{-1}. The minimum displacement of the coordinates for HT computation is 0.01 Angstrom. The DUSHIN correction was turned off and in the vibration correction function computation internal coordinate was used.

Supplementary data:

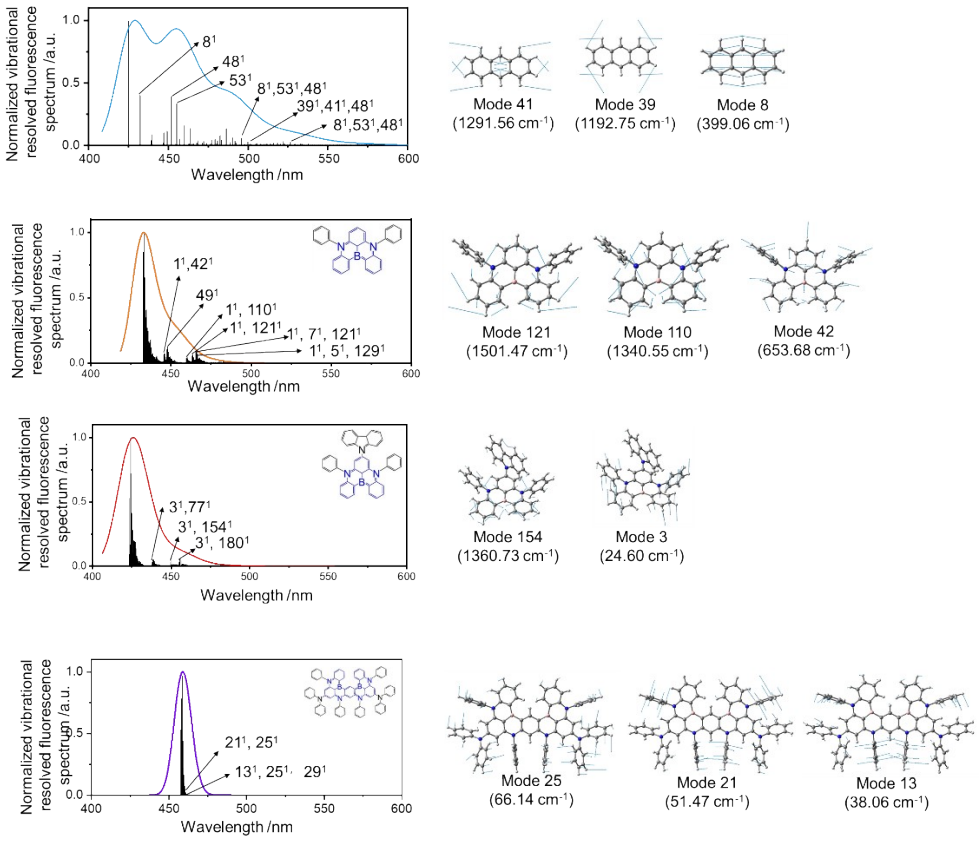

Figure S1. More vibrational modes in the vibrational transitions for **Figure 2** in the main content.

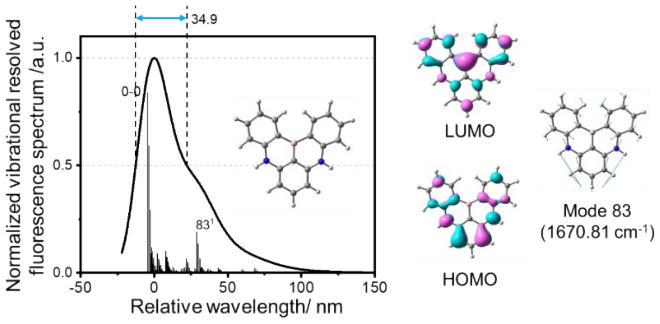

Figure S2. The normalized vibrational resolved fluorescence spectrum of the naked core of DABNA-1 and DABNA-Cz.

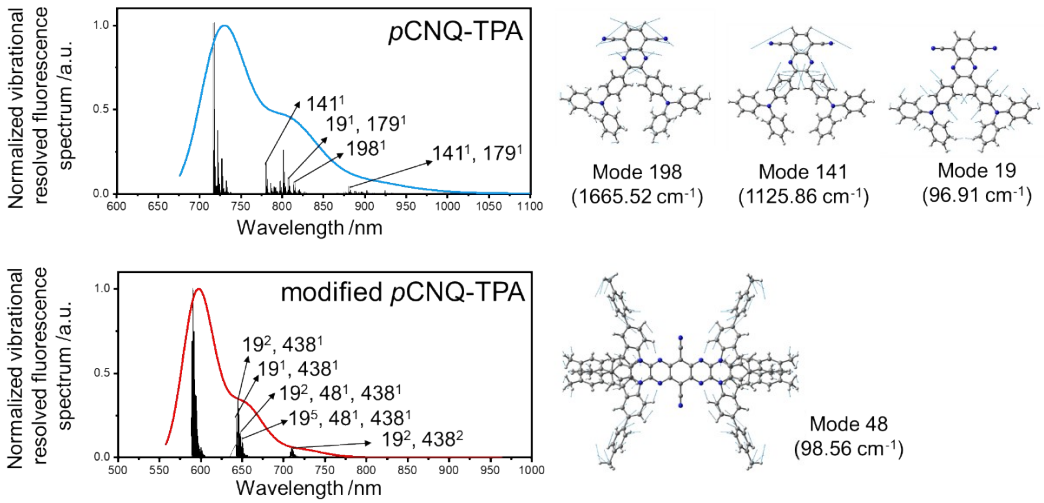

Figure S3. More vibrational modes of the vibrational transitions calculated for *p*CNQ-TPA and modified *p*CNQ-TPA.

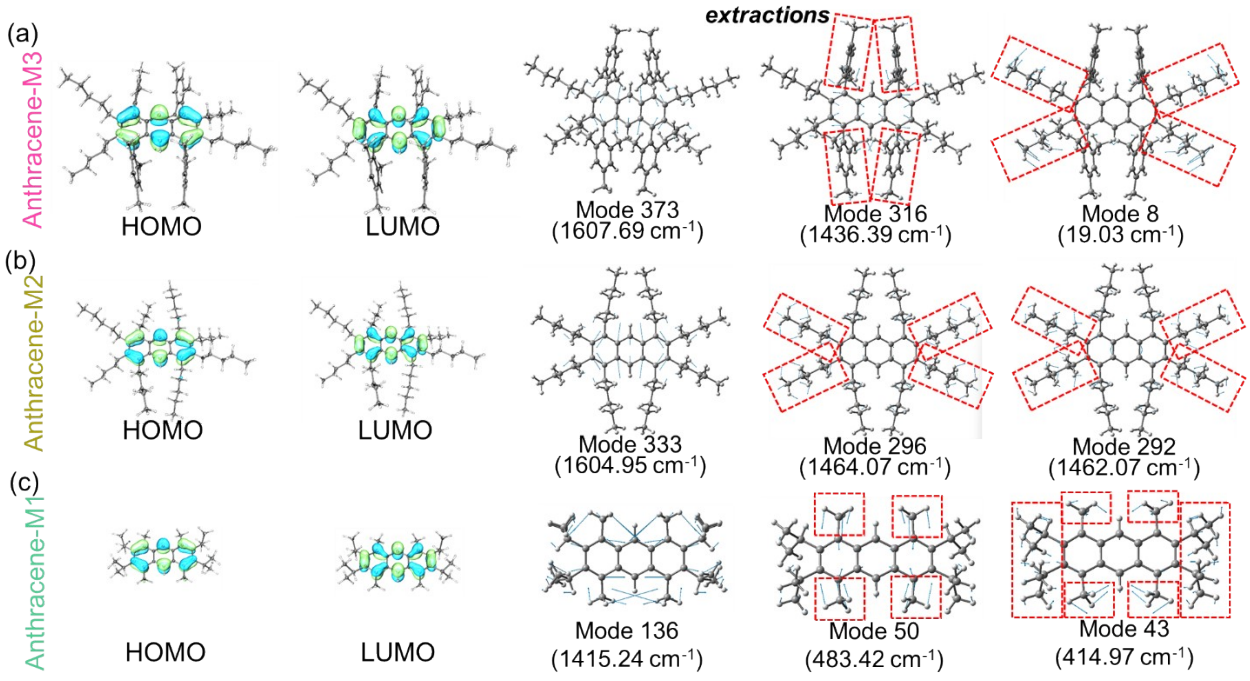

Figure S4. The frontier orbitals and the vibrational modes of the vibrational transitions for the *in-silico* experiment.

Table S1. Parameters for the emissions of the Mr-TADF and the D-A type TADF molecules

	Wavelength /nm		$k_{fluo.}$ /s^{-1}		Transition Dipole moment /debye
	Exp.	Cal.	Exp.	Cal.	Cal.
DANBA-1	462 [a]	437.0	9.6×10^7 [a]	4.1×10^7	4.60
DANBA-Cz	470 [b]	425.9	----	9.7×10^7	5.17

v-DANBA	469 [c]	458.7	2.2×10^{8} [c]	2.0×10^{8}	25.67
*p*CNQ-TPA	724 [d]	729.8	0.83×10^{6} [d]	3.1×10^{7}	18.35
Modified-*p*CNQ-TPA	----	597.2	----	4.0×10^{9}	58.89

a: in film (1 wt% in mCBP).[32]

b: in film (4 wt% in 2,6-DCzppy).[33]

c: in film (1 wt% in DOBNA-OAr).[34] The calculated is much higher than the experimental value because the exciton of *p*CNQ-TPA can be quenched under aggregation.

d: in film (100 wt%).[35]

Table S2. The coordinate of DABNA-1 in S_1 state.

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
B	0.000000	0.000000	-1.362648
C	-0.166741	-1.376486	-2.008793
C	-0.122741	-2.539900	-1.181450
C	-0.387813	-1.623372	-3.384149
C	-0.206537	-3.825357	-1.716709
C	-0.488104	-2.900305	-3.914916
H	-0.509648	-0.783621	-4.047891
C	-0.378736	-4.010868	-3.088963
H	-0.146466	-4.689527	-1.076677
H	-0.651670	-3.027904	-4.977197
H	-0.438946	-5.012066	-3.490920
C	0.166741	1.376486	-2.008793
C	0.122741	2.539900	-1.181450
C	0.387813	1.623372	-3.384149
C	0.206537	3.825357	-1.716709
C	0.488104	2.900305	-3.914916
H	0.509648	0.783621	-4.047891
C	0.378736	4.010868	-3.088963
H	0.146466	4.689527	-1.076677
H	0.651670	3.027904	-4.977197
H	0.438946	5.012066	-3.490920
C	0.000000	0.000000	0.174308
C	0.006681	-1.198785	0.896017
C	-0.006681	1.198785	0.896017
C	0.019223	-1.199805	2.321227
C	-0.019223	1.199805	2.321227
C	0.000000	0.000000	3.008651
H	0.038329	-2.128243	2.866022
H	-0.038329	2.128243	2.866022
H	0.000000	0.000000	4.088882

N	0.000000	2.404728	0.227147
N	0.000000	-2.404728	0.227147
C	0.059087	-3.612671	1.003908
C	-1.114688	-4.208546	1.445089
C	1.292978	-4.171617	1.304680
C	-1.050786	-5.367644	2.208330
H	-2.063720	-3.760240	1.187732
C	1.353144	-5.331473	2.068348
H	2.191642	-3.694614	0.940377
C	0.182566	-5.928953	2.520726
H	-1.962737	-5.831126	2.558104
H	2.313188	-5.766593	2.308704
H	0.230774	-6.830898	3.114952
C	-0.059087	3.612671	1.003908
C	-1.292978	4.171617	1.304680
C	1.114688	4.208546	1.445089
C	-1.353144	5.331473	2.068348
H	-2.191642	3.694614	0.940377
C	1.050786	5.367644	2.208330
H	2.063720	3.760240	1.187732
C	-0.182566	5.928953	2.520726
H	-2.313188	5.766593	2.308704
H	1.962737	5.831126	2.558104
H	-0.230774	6.830898	3.114952

Table S3. The coordinate of DABNA-1 in S_0 state.

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
B	0.000000	0.000000	-1.311956
C	-0.230279	-1.371660	-1.974377
C	-0.170468	-2.529078	-1.158372
C	-0.530658	-1.566097	-3.335155
C	-0.298476	-3.806328	-1.735770
C	-0.693482	-2.816577	-3.895411
H	-0.664352	-0.698919	-3.962412
C	-0.549401	-3.941756	-3.085120
H	-0.218682	-4.689519	-1.123721
H	-0.928817	-2.922547	-4.945266
H	-0.652732	-4.933431	-3.505194
C	0.230279	1.371660	-1.974377
C	0.170468	2.529078	-1.158372
C	0.530658	1.566097	-3.335155
C	0.298476	3.806328	-1.735770
C	0.693482	2.816577	-3.895411

H	0.664352	0.698919	-3.962412
C	0.549401	3.941756	-3.085120
H	0.218682	4.689519	-1.123721
H	0.928817	2.922547	-4.945266
H	0.652732	4.933431	-3.505194
C	0.000000	0.000000	0.198562
C	0.003578	-1.217615	0.921509
C	-0.003578	1.217615	0.921509
C	0.018794	-1.212981	2.321024
C	-0.018794	1.212981	2.321024
C	0.000000	0.000000	2.988665
H	0.032356	-2.132345	2.881270
H	-0.032356	2.132345	2.881270
H	0.000000	0.000000	4.070725
N	0.000000	2.425412	0.225684
N	0.000000	-2.425412	0.225684
C	0.091448	-3.635356	0.991932
C	-1.062587	-4.248578	1.462412
C	1.337597	-4.183302	1.262177
C	-0.968081	-5.417928	2.205544
H	-2.022743	-3.804297	1.241538
C	1.430259	-5.353225	2.005889
H	2.222596	-3.688566	0.887885
C	0.278190	-5.971351	2.477840
H	-1.866024	-5.896273	2.571586
H	2.400785	-5.780897	2.216201
H	0.350929	-6.881850	3.056444
C	-0.091448	3.635356	0.991932
C	-1.337597	4.183302	1.262177
C	1.062587	4.248578	1.462412
C	-1.430259	5.353225	2.005889
H	-2.222596	3.688566	0.887885
C	0.968081	5.417928	2.205544
H	2.022743	3.804297	1.241538
C	-0.278190	5.971351	2.477840
H	-2.400785	5.780897	2.216201
H	1.866024	5.896273	2.571586
H	-0.350929	6.881850	3.056444

Table S4. The coordinate of DABNA-Cz in S_1 state.

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	-1.270389	0.000000	0.000000
C	-0.570296	-1.194182	-0.184485

C	-0.570296	1.194182	0.184485
C	0.854459	-1.194534	-0.128057
H	-1.122108	-2.108906	-0.376645
N	-2.681784	0.000000	0.000001
C	0.854459	1.194534	0.128057
H	-1.122108	2.108906	0.376646
N	1.523631	-2.404815	-0.233333
C	1.587380	0.000000	0.000000
C	-3.500718	0.905780	-0.691119
C	-3.500718	-0.905780	0.691121
N	1.523631	2.404815	0.233332
C	2.935725	-2.534479	-0.336944
C	0.727061	-3.603592	-0.249161
B	3.122759	0.000000	-0.000001
C	-3.150072	1.962545	-1.538703
C	-4.859778	0.577167	-0.439009
C	-3.150071	-1.962545	1.538705
C	-4.859778	-0.577167	0.439011
C	2.935725	2.534479	0.336943
C	0.727061	3.603592	0.249161
C	3.472901	-3.821387	-0.493757
C	3.770230	-1.365879	-0.283788
C	0.310292	-4.161461	0.961603
C	0.350224	-4.176867	-1.465696
C	3.770230	1.365879	0.283786
C	-4.183272	2.702118	-2.115540
H	-2.108946	2.204512	-1.748757
C	-5.877620	1.335667	-1.030769
C	-4.183271	-2.702119	2.115542
H	-2.108946	-2.204512	1.748758
C	-5.877619	-1.335667	1.030772
C	3.472901	3.821387	0.493756
C	0.310291	4.161461	-0.961602
C	0.350225	4.176867	1.465696
C	4.853833	-3.997226	-0.663399
H	2.822884	-4.693514	-0.491075
C	5.152216	-1.600967	-0.509266
C	-0.507495	-5.294581	0.953362
H	0.625751	-3.697513	1.897232
C	-0.464918	-5.311211	-1.468273
H	0.692683	-3.723583	-2.396816
C	5.152217	1.600968	0.509264
C	-5.533802	2.399277	-1.863586
H	-3.932774	3.533394	-2.777647

H	-6.925291	1.091826	-0.843281
C	-5.533801	-2.399277	1.863589
H	-3.932772	-3.533394	2.777649
H	-6.925290	-1.091827	0.843284
C	4.853833	3.997226	0.663397
H	2.822884	4.693514	0.491074
C	-0.507496	5.294581	-0.953361
H	0.625749	3.697513	-1.897233
C	-0.464918	5.311211	1.468273
H	0.692684	3.723583	2.396815
C	5.686753	-2.877119	-0.692879
H	5.259659	-5.003011	-0.782197
H	5.823631	-0.746456	-0.563317
C	-0.896657	-5.868475	-0.260164
H	-0.841989	-5.728176	1.897665
H	-0.769264	-5.756824	-2.417126
C	5.686753	2.877120	0.692876
H	5.823632	0.746456	0.563314
H	-6.316867	3.000535	-2.328917
H	-6.316865	-3.000535	2.328920
H	5.259659	5.003011	0.782195
C	-0.896657	5.868475	0.260165
H	-0.841991	5.728176	-1.897665
H	-0.769263	5.756824	2.417127
H	6.760845	-2.995967	-0.854798
H	-1.539104	-6.750987	-0.265409
H	6.760845	2.995967	0.854794
H	-1.539104	6.750987	0.265410

Table S5. The coordinate of DABNA-Cz in S_0 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	-1.259106	0.000000	0.000000
C	-0.580386	-1.209894	-0.157199
C	-0.580386	1.209894	0.157200
C	0.824151	-1.211865	-0.131367
H	-1.146138	-2.120956	-0.320723
N	-2.675199	0.000000	0.000001
C	0.824151	1.211865	0.131366
H	-1.146138	2.120956	0.320724
N	1.514387	-2.420319	-0.242657
C	1.556352	0.000000	0.000000
C	-3.493757	0.885810	-0.715141
C	-3.493757	-0.885810	0.715143

N	1.514387	2.420319	0.242656
C	2.906412	-2.515322	-0.403271
C	0.732185	-3.627020	-0.227150
B	3.070837	0.000000	-0.000001
C	-3.145124	1.916463	-1.595932
C	-4.853367	0.563573	-0.455949
C	-3.145123	-1.916463	1.595934
C	-4.853367	-0.563573	0.455952
C	2.906412	2.515322	0.403270
C	0.732185	3.627020	0.227150
C	3.479040	-3.787940	-0.629890
C	3.731363	-1.353819	-0.351173
C	0.400871	-4.211749	0.997190
C	0.279640	-4.185758	-1.424819
C	3.731363	1.353819	0.351171
C	-4.179114	2.635471	-2.196436
H	-2.103583	2.151692	-1.809347
C	-5.872281	1.301437	-1.071777
C	-4.179113	-2.635471	2.196438
H	-2.103582	-2.151692	1.809348
C	-5.872281	-1.301437	1.071780
C	3.479040	3.787940	0.629888
C	0.400870	4.211749	-0.997191
C	0.279640	4.185758	1.424819
C	4.839759	-3.911453	-0.871897
H	2.852518	-4.677463	-0.631793
C	5.102932	-1.533701	-0.647231
C	-0.392211	-5.361409	1.023305
H	0.764296	-3.754621	1.918733
C	-0.510473	-5.337312	-1.395217
H	0.547093	-3.708497	-2.368614
C	5.102933	1.533702	0.647229
C	-5.529799	2.339066	-1.936907
H	-3.929195	3.446337	-2.883830
H	-6.919649	1.061090	-0.877605
C	-5.529798	-2.339067	1.936909
H	-3.929193	-3.446338	2.883832
H	-6.919648	-1.061091	0.877608
C	4.839760	3.911453	0.871894
H	2.852518	4.677463	0.631791
C	-0.392212	5.361409	-1.023305
H	0.764295	3.754621	-1.918733
C	-0.510472	5.337312	1.395217
H	0.547094	3.708497	2.368614

C	5.662323	-2.777110	-0.907876
H	5.260044	-4.903343	-1.052808
H	5.743187	-0.654125	-0.695647
C	-0.848914	-5.924295	-0.172152
H	-0.655172	-5.817549	1.979635
H	-0.867549	-5.773851	-2.329908
C	5.662323	2.777111	0.907873
H	5.743187	0.654125	0.695644
H	-6.313394	2.924287	-2.421669
H	-6.313392	-2.924287	2.421672
H	5.260044	4.903343	1.052806
C	-0.848915	5.924295	0.172153
H	-0.655173	5.817549	-1.979635
H	-0.867548	5.773851	2.329909
H	6.725763	-2.870339	-1.135461
H	-1.471512	-6.820777	-0.150762
H	6.725763	2.870340	1.135458
H	-1.471512	6.820777	0.150762

Table S6. The coordinate of *v*-DABNA in S_1 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	1.215728	-0.314716	0.017691
N	2.400972	-1.061500	-0.013308
C	-0.001211	-0.996611	-0.114318
C	3.680100	-0.497413	0.038862
C	2.299205	-2.489482	-0.144694
C	1.241011	1.102757	0.191598
C	-1.217871	-0.303430	-0.156398
H	-0.000875	-2.077084	-0.183932
C	4.798784	-1.318910	-0.148440
C	3.814028	0.900430	0.268543
C	2.327515	-3.290090	0.999072
C	2.159112	-3.067486	-1.408829
C	-0.002501	1.748215	0.088483
B	2.600615	1.791138	0.441604
N	-2.402665	-1.047531	-0.243685
C	-1.244586	1.123635	-0.111955
C	6.082693	-0.764692	-0.051699
H	4.687617	-2.375931	-0.366502
C	5.131536	1.429898	0.323715
C	2.210412	-4.676360	0.877483
H	2.438460	-2.815356	1.974854
C	2.035835	-4.453353	-1.526451

H	2.137441	-2.421516	-2.287486
H	-0.004339	2.828258	0.174699
C	2.908550	3.259864	0.829504
C	-3.682300	-0.485293	-0.182164
C	-2.295304	-2.480659	-0.282407
B	-2.608245	1.839593	-0.217246
C	6.257103	0.601282	0.198488
N	7.214835	-1.593434	-0.213610
N	5.309039	2.804121	0.510100
C	2.060291	-5.258742	-0.384136
H	2.232638	-5.302996	1.771127
H	1.919243	-4.905481	-2.513254
C	1.943537	4.214541	1.228178
C	4.264258	3.700438	0.789851
C	-4.802271	-1.326469	-0.175991
C	-3.818708	0.930983	-0.152602
C	-2.143520	-3.131549	-1.508226
C	-2.322713	-3.211740	0.907930
C	-2.922053	3.349517	-0.366825
H	7.261201	1.001267	0.286852
C	7.167668	-2.960978	0.163919
C	8.421437	-1.064059	-0.743732
C	6.654182	3.304260	0.429172
H	1.963283	-6.342111	-0.477641
C	2.256675	5.538821	1.504750
H	0.909581	3.895177	1.345575
C	4.582624	5.055479	1.038798
C	-6.079561	-0.766853	-0.036155
H	-4.696665	-2.403257	-0.257201
C	-5.133953	1.461151	-0.056954
C	-2.006733	-4.521270	-1.541892
H	-2.122647	-2.538697	-2.423632
C	-2.193190	-4.601133	0.870325
H	-2.442793	-2.680821	1.853107
C	-1.965686	4.351047	-0.655576
C	-4.276287	3.775894	-0.237444
C	7.724098	-3.941939	-0.671688
C	6.565460	-3.350010	1.371720
C	9.651239	-1.371108	-0.141545
C	8.399142	-0.225655	-1.870207
C	7.424465	3.436169	1.587153
C	7.198616	3.610048	-0.820177
C	3.587783	5.959468	1.384058
H	1.476767	6.239192	1.809247

H	5.614025	5.395689	0.971810
C	-6.251721	0.619220	0.050750
N	-7.209702	-1.613167	0.017219
N	-5.313280	2.847784	-0.042635
C	-2.030271	-5.256689	-0.353690
H	-1.880098	-5.030588	-2.499179
H	-2.216357	-5.173305	1.799669
C	-2.286510	5.698428	-0.756209
H	-0.933866	4.052759	-0.833000
C	-4.604032	5.148815	-0.321254
C	7.678457	-5.286659	-0.302549
H	8.191202	-3.640149	-1.609990
C	6.505807	-4.698177	1.722741
H	6.136537	-2.588311	2.023193
C	10.836346	-0.847470	-0.659639
H	9.668360	-2.021697	0.733745
C	9.585965	0.309949	-2.368778
H	7.443902	0.011052	-2.339348
C	8.746994	3.875560	1.492566
H	6.979951	3.185410	2.551287
C	8.523037	4.043151	-0.912192
H	6.579576	3.491319	-1.710467
H	3.857859	7.000372	1.576684
H	-7.249975	1.022530	0.180404
C	-7.112161	-2.909462	0.586452
C	-8.462157	-1.166928	-0.481013
C	-6.662718	3.331767	0.063424
H	-1.922526	-6.342731	-0.381334
C	-3.617699	6.093366	-0.568983
H	-1.513635	6.435441	-0.981982
H	-5.636349	5.472523	-0.204959
C	7.063681	-5.674604	0.891467
H	8.115012	-6.038800	-0.963318
H	6.028904	-4.986079	2.662174
C	10.811560	0.001246	-1.770040
H	11.786062	-1.094089	-0.179943
H	9.552475	0.966042	-3.241255
C	9.298533	4.175578	0.243319
H	9.350903	3.976208	2.396539
H	8.951937	4.273504	-1.889302
C	-7.724962	-4.004164	-0.043099
C	-6.402873	-3.114532	1.781440
C	-9.635385	-1.386137	0.257111
C	-8.541644	-0.497650	-1.713255

C	-7.185455	3.662504	1.315020
C	-7.456297	3.428672	-1.082700
H	-3.895205	7.148038	-0.633716
H	7.020458	-6.728529	1.172454
H	11.739393	0.417940	-2.166368
H	10.335243	4.509924	0.170096
C	-7.629345	-5.279092	0.515550
H	-8.275051	-3.845596	-0.971500
C	-6.295430	-4.395454	2.321864
H	-5.930526	-2.263988	2.273484
C	-10.865054	-0.943270	-0.231753
H	-9.573637	-1.904672	1.214697
C	-9.771692	-0.040775	-2.184735
H	-7.630357	-0.330188	-2.287920
C	-8.510663	4.092800	1.420094
H	-6.548149	3.573482	2.195887
C	-8.782122	3.851939	-0.973803
H	-7.027794	3.156613	-2.048191
C	-6.909340	-5.485032	1.695944
H	-8.110655	-6.121347	0.013703
H	-5.736883	-4.540062	3.249290
C	-10.941076	-0.262424	-1.450164
H	-11.769662	-1.119737	0.354268
H	-9.817475	0.482316	-3.142472
C	-9.310564	4.184431	0.277366
H	-8.921246	4.350266	2.398436
H	-9.406065	3.916886	-1.867148
H	-6.828252	-6.485426	2.125137
H	-11.903288	0.091422	-1.825023
H	-10.348524	4.512243	0.362058

Table S7. The coordinate of *v*-DABNA in S_0 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	1.215728	-0.314716	0.017691
N	2.400972	-1.061500	-0.013308
C	-0.001211	-0.996611	-0.114318
C	3.680100	-0.497413	0.038862
C	2.299205	-2.489482	-0.144694
C	1.241011	1.102757	0.191598
C	-1.217871	-0.303430	-0.156398
H	-0.000875	-2.077084	-0.183932
C	4.798784	-1.318910	-0.148440
C	3.814028	0.900430	0.268543

C	2.327515	-3.290090	0.999072
C	2.159112	-3.067486	-1.408829
C	-0.002501	1.748215	0.088483
B	2.600615	1.791138	0.441604
N	-2.402665	-1.047531	-0.243685
C	-1.244586	1.123635	-0.111955
C	6.082693	-0.764692	-0.051699
H	4.687617	-2.375931	-0.366502
C	5.131536	1.429898	0.323715
C	2.210412	-4.676360	0.877483
H	2.438460	-2.815356	1.974854
C	2.035835	-4.453353	-1.526451
H	2.137441	-2.421516	-2.287486
H	-0.004339	2.828258	0.174699
C	2.908550	3.259864	0.829504
C	-3.682300	-0.485293	-0.182164
C	-2.295304	-2.480659	-0.282407
B	-2.608245	1.839593	-0.217246
C	6.257103	0.601282	0.198488
N	7.214835	-1.593434	-0.213610
N	5.309039	2.804121	0.510100
C	2.060291	-5.258742	-0.384136
H	2.232638	-5.302996	1.771127
H	1.919243	-4.905481	-2.513254
C	1.943537	4.214541	1.228178
C	4.264258	3.700438	0.789851
C	-4.802271	-1.326469	-0.175991
C	-3.818708	0.930983	-0.152602
C	-2.143520	-3.131549	-1.508226
C	-2.322713	-3.211740	0.907930
C	-2.922053	3.349517	-0.366825
H	7.261201	1.001267	0.286852
C	7.167668	-2.960978	0.163919
C	8.421437	-1.064059	-0.743732
C	6.654182	3.304260	0.429172
H	1.963283	-6.342111	-0.477641
C	2.256675	5.538821	1.504750
H	0.909581	3.895177	1.345575
C	4.582624	5.055479	1.038798
C	-6.079561	-0.766853	-0.036155
H	-4.696665	-2.403257	-0.257201
C	-5.133953	1.461151	-0.056954
C	-2.006733	-4.521270	-1.541892
H	-2.122647	-2.538697	-2.423632

C	-2.193190	-4.601133	0.870325
H	-2.442793	-2.680821	1.853107
C	-1.965686	4.351047	-0.655576
C	-4.276287	3.775894	-0.237444
C	7.724098	-3.941939	-0.671688
C	6.565460	-3.350010	1.371720
C	9.651239	-1.371108	-0.141545
C	8.399142	-0.225655	-1.870207
C	7.424465	3.436169	1.587153
C	7.198616	3.610048	-0.820177
C	3.587783	5.959468	1.384058
H	1.476767	6.239192	1.809247
H	5.614025	5.395689	0.971810
C	-6.251721	0.619220	0.050750
N	-7.209702	-1.613167	0.017219
N	-5.313280	2.847784	-0.042635
C	-2.030271	-5.256689	-0.353690
H	-1.880098	-5.030588	-2.499179
H	-2.216357	-5.173305	1.799669
C	-2.286510	5.698428	-0.756209
H	-0.933866	4.052759	-0.833000
C	-4.604032	5.148815	-0.321254
C	7.678457	-5.286659	-0.302549
H	8.191202	-3.640149	-1.609990
C	6.505807	-4.698177	1.722741
H	6.136537	-2.588311	2.023193
C	10.836346	-0.847470	-0.659639
H	9.668360	-2.021697	0.733745
C	9.585965	0.309949	-2.368778
H	7.443902	0.011052	-2.339348
C	8.746994	3.875560	1.492566
H	6.979951	3.185410	2.551287
C	8.523037	4.043151	-0.912192
H	6.579576	3.491319	-1.710467
H	3.857859	7.000372	1.576684
H	-7.249975	1.022530	0.180404
C	-7.112161	-2.909462	0.586452
C	-8.462157	-1.166928	-0.481013
C	-6.662718	3.331767	0.063424
H	-1.922526	-6.342731	-0.381334
C	-3.617699	6.093366	-0.568983
H	-1.513635	6.435441	-0.981982
H	-5.636349	5.472523	-0.204959
C	7.063681	-5.674604	0.891467

H	8.115012	-6.038800	-0.963318
H	6.028904	-4.986079	2.662174
C	10.811560	0.001246	-1.770040
H	11.786062	-1.094089	-0.179943
H	9.552475	0.966042	-3.241255
C	9.298533	4.175578	0.243319
H	9.350903	3.976208	2.396539
H	8.951937	4.273504	-1.889302
C	-7.724962	-4.004164	-0.043099
C	-6.402873	-3.114532	1.781440
C	-9.635385	-1.386137	0.257111
C	-8.541644	-0.497650	-1.713255
C	-7.185455	3.662504	1.315020
C	-7.456297	3.428672	-1.082700
H	-3.895205	7.148038	-0.633716
H	7.020458	-6.728529	1.172454
H	11.739393	0.417940	-2.166368
H	10.335243	4.509924	0.170096
C	-7.629345	-5.279092	0.515550
H	-8.275051	-3.845596	-0.971500
C	-6.295430	-4.395454	2.321864
H	-5.930526	-2.263988	2.273484
C	-10.865054	-0.943270	-0.231753
H	-9.573637	-1.904672	1.214697
C	-9.771692	-0.040775	-2.184735
H	-7.630357	-0.330188	-2.287920
C	-8.510663	4.092800	1.420094
H	-6.548149	3.573482	2.195887
C	-8.782122	3.851939	-0.973803
H	-7.027794	3.156613	-2.048191
C	-6.909340	-5.485032	1.695944
H	-8.110655	-6.121347	0.013703
H	-5.736883	-4.540062	3.249290
C	-10.941076	-0.262424	-1.450164
H	-11.769662	-1.119737	0.354268
H	-9.817475	0.482316	-3.142472
C	-9.310564	4.184431	0.277366
H	-8.921246	4.350266	2.398436
H	-9.406065	3.916886	-1.867148
H	-6.828252	-6.485426	2.125137
H	-11.903288	0.091422	-1.825023
H	-10.348524	4.512243	0.362058

Table S8. The coordinate of *p*CNQ-TPA in S_1 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	-1.565065	1.384726	0.015086
C	-1.296239	0.298017	-0.841934
C	-2.769425	1.360386	0.747239
C	-2.147562	-0.784737	-0.916990
H	-0.418663	0.329566	-1.487442
C	-0.699982	2.572198	0.092797
C	-3.624139	0.279539	0.684682
H	-3.005589	2.218952	1.374390
C	-3.325345	-0.822448	-0.142677
H	-1.933643	-1.600657	-1.606777
C	0.694629	2.573681	-0.092583
N	-1.372342	3.724557	0.300611
H	-4.532922	0.269780	1.285763
N	-4.187433	-1.918262	-0.214657
C	1.562216	1.388030	-0.014992
N	1.364549	3.727481	-0.300284
C	-0.701238	4.874401	0.191853
C	-5.590987	-1.748473	-0.059747
C	-3.676569	-3.223940	-0.441355
C	2.766630	1.366311	-0.747138
C	1.295673	0.300661	0.841903
C	0.691013	4.875892	-0.191419
C	-1.357874	6.121073	0.421648
C	-6.316823	-2.621969	0.756628
C	-6.254453	-0.715063	-0.730034
C	-4.294847	-4.070702	-1.367617
C	-2.562322	-3.678985	0.272597
C	3.623616	0.287259	-0.684698
H	3.000991	2.225445	-1.374188
C	2.149272	-0.780308	0.916839
H	0.418030	0.330292	1.487411
C	1.345008	6.123973	-0.421096
C	-0.668614	7.325008	0.214552
C	-2.720189	6.121935	0.846659
C	-7.689908	-2.459970	0.897778
H	-5.797414	-3.424195	1.281634
C	-7.625962	-0.554017	-0.572585
H	-5.689471	-0.040873	-1.374446
C	-3.802335	-5.353941	-1.573368
H	-5.161850	-3.714553	-1.924667
C	-2.071616	-4.960917	0.053615

H	-2.089780	-3.023567	1.004671
C	3.327134	-0.815451	0.142528
H	4.532425	0.279481	-1.285770
H	1.937066	-1.596758	1.606530
C	0.653201	7.326427	-0.213883
C	2.707317	6.127760	-0.846109
H	-1.186291	8.268394	0.386443
N	-3.826153	6.146162	1.197516
C	-8.349930	-1.425103	0.238447
H	-8.247648	-3.143515	1.539975
H	-8.134075	0.255844	-1.098273
C	-2.688573	-5.804862	-0.867724
H	-4.290189	-6.005375	-2.300240
H	-1.206376	-5.306330	0.622199
N	4.191526	-1.909460	0.214383
H	1.168881	8.270923	-0.385683
N	3.813226	6.154363	-1.196966
H	-9.426832	-1.297575	0.356530
H	-2.305881	-6.813105	-1.032634
C	5.594725	-1.736680	0.059554
C	3.683409	-3.216241	0.440881
C	6.255976	-0.701979	0.730037
C	6.322439	-2.608503	-0.756936
C	4.303476	-4.061853	1.366998
C	2.570105	-3.673510	-0.273122
C	7.627148	-0.538007	0.572673
H	5.689543	-0.029090	1.374536
C	7.695185	-2.443578	-0.898001
H	5.804750	-3.411739	-1.282096
C	3.813660	-5.346155	1.572553
H	5.169739	-3.703978	1.924093
C	2.082091	-4.956502	-0.054334
H	2.096173	-3.018971	-1.005084
C	8.352991	-1.407426	-0.238470
H	8.133525	0.272840	1.098516
H	8.254396	-3.125836	-1.540288
C	2.700833	-5.799299	0.866858
H	4.302893	-5.996680	2.299312
H	1.217566	-5.303636	-0.622958
H	9.429625	-1.277602	-0.356487
H	2.320259	-6.808370	1.031614

Table S9. The coordinate of *p*CNQ-TPA in S_0 state

	Coordinates /Å		

Elements	X	Y	Z
C	-1.572865	1.413502	0.003291
C	-1.300395	0.348529	-0.864216
C	-2.7445	1.356166	0.76808
C	-2.155497	-0.738669	-0.951884
H	-0.419602	0.37633	-1.505344
C	-0.728503	2.630106	0.064964
C	-3.589195	0.259682	0.707885
H	-2.984267	2.19103	1.426367
C	-3.308042	-0.809896	-0.155211
H	-1.935255	-1.545344	-1.650728
C	0.723019	2.63164	-0.064791
N	-1.378596	3.761607	0.217593
H	-4.481249	0.228096	1.332943
N	-4.16221	-1.92494	-0.22805
C	1.56994	1.416809	-0.003244
N	1.37073	3.764523	-0.217293
C	-0.694662	4.926238	0.146705
C	-5.565364	-1.772294	-0.056304
C	-3.630651	-3.226027	-0.436575
C	2.741706	1.362029	-0.768019
C	1.299694	0.351161	0.864131
C	0.684347	4.927705	-0.146277
C	-1.376607	6.164586	0.317121
C	-6.273044	-2.645487	0.775354
C	-6.254848	-0.755507	-0.724942
C	-4.226322	-4.090054	-1.361021
C	-2.51895	-3.664958	0.289874
C	3.588704	0.267318	-0.707938
H	2.979728	2.197474	-1.426201
C	2.157078	-0.734247	0.951683
H	0.418834	0.377035	1.505248
C	1.363686	6.167503	-0.316562
C	-0.691737	7.354858	0.163315
C	-2.776683	6.166608	0.638699
C	-7.648269	-2.504739	0.928728
H	-5.737759	-3.438501	1.298728
C	-7.626782	-0.609785	-0.551334
H	-5.707101	-0.076473	-1.379416
C	-3.720445	-5.371882	-1.548125
H	-5.093233	-3.749861	-1.928568
C	-2.009228	-4.942934	0.086281
H	-2.05584	-2.997227	1.017159
C	3.309785	-0.802953	0.155023

H	4.480836	0.237682	-1.332981
H	1.938519	-1.54147	1.650424
C	0.676312	7.356314	-0.162631
C	2.763754	6.172504	-0.63814
H	-1.219386	8.299572	0.290663
N	-3.902265	6.207941	0.903068
C	-8.331804	-1.48479	0.27177
H	-8.188261	-3.19444	1.579998
H	-8.151139	0.190504	-1.076547
C	-2.608185	-5.804686	-0.829946
H	-4.196865	-6.035803	-2.271755
H	-1.142625	-5.270338	0.663524
N	4.166303	-1.916202	0.227746
H	1.201972	8.30215	-0.289878
N	3.889246	6.216233	-0.902506
H	-9.409322	-1.372146	0.400147
H	-2.212394	-6.810128	-0.981287
C	5.569142	-1.76055	0.05613
C	3.637487	-3.218436	0.436072
C	6.25641	-0.742402	0.72498
C	6.278742	-2.632104	-0.775609
C	4.234979	-4.081352	1.360382
C	2.526709	-3.659596	-0.290439
C	7.628045	-0.593735	0.551503
H	5.707168	-0.064635	1.379516
C	7.653677	-2.488408	-0.928853
H	5.745185	-3.426172	-1.29915
C	3.731803	-5.36427	1.54729
H	5.101175	-3.739425	1.927979
C	2.019678	-4.938674	-0.087039
H	2.062188	-2.992734	-1.01762
C	8.33499	-1.467111	-0.271681
H	8.150657	0.207585	1.076882
H	8.195185	-3.176857	-1.580189
C	2.620452	-5.799305	0.829051
H	4.209624	-6.027298	2.270817
H	1.153763	-5.26781	-0.664329
H	9.412276	-1.352155	-0.399956
H	2.22678	-6.805601	0.98024

Table S10. The coordinate of modified *p*CNQ-TPA in S_1 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	1.225901	-0.682017	-0.234076

C	-0.000263	-1.361657	-0.431456
C	1.226003	0.681635	0.235271
C	-1.226337	-0.681939	-0.233872
C	-0.000332	-2.727651	-0.839311
N	2.386391	-1.286721	-0.533832
C	-0.000068	1.361365	0.432822
N	2.386604	1.286249	0.534821
C	-1.226236	0.681724	0.235455
N	-2.386934	-1.286558	-0.533411
N	-0.000367	-3.848619	-1.135655
C	3.517057	-0.631847	-0.325978
C	-0.000006	2.727408	0.840513
C	3.517180	0.631298	0.326753
N	-2.386724	1.286454	0.535140
C	-3.517516	-0.631596	-0.325380
N	4.688208	-1.256954	-0.783584
N	0.000015	3.848429	1.136659
N	4.688489	1.256291	0.784098
C	-3.517394	0.631576	0.327276
N	-4.688813	-1.256597	-0.782745
C	4.981967	-2.617845	-0.627914
C	5.737027	-0.659509	-1.497653
C	4.982378	2.617150	0.628326
C	5.737412	0.658743	1.497936
N	-4.688552	1.256798	0.784730
C	-4.982773	-2.617425	-0.626837
C	-5.737671	-0.659083	-1.496698
C	4.240304	-3.632086	-0.019456
C	6.252526	-2.877113	-1.179545
C	5.854892	0.632140	-2.007908
C	6.733047	-1.625038	-1.740890
C	4.240696	3.631466	0.020025
C	6.253100	2.876274	1.179642
C	5.855257	-0.632906	2.008193
C	6.733602	1.624161	1.740906
C	-4.982219	2.617674	0.628808
C	-5.737572	0.659478	1.498598
C	-4.241166	-3.631705	-0.018384
C	-6.253476	-2.876554	-1.178189
C	-5.855431	0.632518	-2.007095
C	-6.733892	-1.624483	-1.739617
C	4.805028	-4.897842	0.038090
H	3.234455	-3.451326	0.350784
C	6.796374	-4.153594	-1.110742

C	7.003992	0.948931	-2.719326
H	5.080280	1.382847	-1.865329
C	7.876282	-1.285947	-2.454348
C	4.805570	4.897149	-0.037700
H	3.234727	3.450824	-0.349950
C	6.797093	4.152694	1.110670
C	7.004495	-0.949814	2.719335
H	5.080515	-1.383524	1.865834
C	7.876979	1.284950	2.454096
C	-4.240450	3.631746	0.020233
C	-6.252974	2.877044	1.179988
C	-5.855572	-0.632087	2.009042
C	-6.733667	1.625046	1.741386
C	-4.806096	-4.897355	0.039452
H	-3.235209	-3.451064	0.351627
C	-6.797531	-4.152945	-1.109100
C	-7.004610	0.949396	-2.718348
H	-5.080662	1.383114	-1.864758
C	-7.877215	-1.285295	-2.452908
C	6.077820	-5.184850	-0.494675
H	4.221610	-5.707372	0.477893
H	7.792063	-4.345557	-1.512950
C	8.031630	0.014292	-2.947127
H	7.119191	1.965689	-3.096195
H	8.635104	-2.042116	-2.660680
C	6.078527	5.184012	0.494747
H	4.222150	5.706744	-0.477385
H	7.792900	4.344545	1.512640
C	8.032298	-0.015288	2.946864
H	7.119666	-1.966573	3.096209
H	8.635940	2.041037	2.660222
C	-4.805251	4.897461	-0.037877
H	-3.234551	3.450884	-0.349819
C	-6.796912	4.153426	1.110559
C	-7.004873	-0.948756	2.720186
H	-5.080914	-1.382812	1.866813
C	-7.877093	1.286088	2.454581
C	-6.079042	-5.184223	-0.493026
H	-4.222734	-5.706925	0.479259
H	-7.793328	-4.344796	-1.511096
C	-8.032439	0.014891	-2.945834
H	-7.119719	1.966117	-3.095348
H	-8.636206	-2.041365	-2.658987
C	6.639837	-6.554066	-0.410173

C	9.246337	0.395361	-3.708700
C	6.640693	6.553163	0.410065
C	9.247150	-0.396485	3.708149
C	-6.078085	5.184622	0.494684
H	-4.221672	5.706712	-0.477997
H	-7.792821	4.345608	1.512100
C	-8.032579	-0.014080	2.947540
H	-7.120170	-1.965448	3.097200
H	-8.635954	2.042304	2.660588
C	-6.641273	-6.553340	-0.408213
C	-9.247227	0.396059	-3.707240
C	6.433779	-7.354147	0.718896
C	7.399327	-7.092805	-1.458372
C	9.173493	1.249669	-4.813708
C	10.509450	-0.092507	-3.346129
C	6.434589	7.353177	-0.719041
C	7.400385	7.091893	1.458119
C	9.174471	-1.250717	4.813225
C	10.510239	0.091175	3.345219
C	-6.639724	6.554011	0.410503
C	-9.247486	-0.395012	3.708848
C	-6.435224	-7.353246	0.720977
C	-7.400958	-7.092150	-1.456234
C	-9.174414	1.250015	-4.812519
C	-10.510382	-0.091368	-3.344232
C	6.965449	-8.637259	0.796730
H	5.867550	-6.958580	1.563766
C	7.926927	-8.373866	-1.376387
H	7.556880	-6.506411	-2.365226
C	10.315790	1.600777	-5.526283
H	8.203288	1.628571	-5.139522
C	11.646209	0.260548	-4.060335
H	10.604704	-0.741033	-2.473358
C	6.966404	8.636219	-0.797048
H	5.868209	6.957601	-1.563807
C	7.928136	8.372884	1.375961
H	7.557994	6.505544	2.364993
C	10.316903	-1.601950	5.525523
H	8.204296	-1.629465	5.139309
C	11.647133	-0.262000	4.059152
H	10.605358	0.739631	2.472381
C	-7.397563	7.093182	1.455658
C	-6.431686	7.354786	-0.721439
C	-9.174965	-1.249278	4.813912

C	-10.510475	0.092957	3.345973
C	-6.967091	-8.636262	0.799103
H	-5.868830	-6.957617	1.565709
C	-7.928760	-8.373110	-1.373957
H	-7.558504	-6.505895	-2.363179
C	-10.316785	1.601210	-5.524937
H	-8.204178	1.628554	-5.138668
C	-11.647215	0.261769	-4.058282
H	-10.605596	-0.739613	-2.471247
C	7.720519	-9.173019	-0.247218
H	6.794157	-9.233670	1.695809
H	8.506658	-8.768334	-2.214582
C	11.572819	1.114700	-5.165347
H	10.224753	2.263221	-6.390160
H	12.617705	-0.130037	-3.747243
C	7.721671	9.171974	0.246760
H	6.795081	9.232574	-1.696159
H	8.508039	8.767341	2.214041
C	11.573907	-1.116071	5.164236
H	10.225995	-2.264338	6.389456
H	12.618606	0.128421	3.745780
C	-7.925207	8.377597	1.372055
H	-7.556447	6.508749	2.363508
C	-6.960955	8.635333	-0.800512
H	-5.864772	6.957144	-1.564914
C	-10.317451	-1.600249	5.526248
H	-8.204869	-1.628244	5.139974
C	-11.647424	-0.259966	4.059938
H	-10.605482	0.741464	2.473163
C	-7.722365	-9.172088	-0.244661
H	-6.795789	-9.232540	1.698268
H	-8.508639	-8.767640	-2.212020
C	-11.573857	1.115569	-5.163567
H	-10.225775	2.263361	-6.389042
H	-12.618740	-0.128469	-3.744850
C	8.289225	-10.564576	-0.174529
C	12.812884	1.491620	-5.930740
C	8.290469	10.563487	0.173910
C	12.814109	-1.493073	5.929370
C	-7.717996	9.173794	0.245033
H	-8.504893	8.773392	2.209133
H	-6.788394	9.230855	-1.700422
C	-11.574356	-1.114076	5.165005
H	-10.226665	-2.262652	6.390181

H	-12.618812	0.130703	3.746619
C	-8.291342	-10.563518	-0.171635
C	-12.814000	1.492561	-5.928803
H	9.374757	-10.563124	-0.358371
H	7.833384	-11.219839	-0.933852
H	8.113204	-11.020144	0.809633
H	13.319721	0.600575	-6.333209
H	13.537422	2.011374	-5.284203
H	12.578532	2.155471	-6.774194
H	9.375861	10.562096	0.358549
H	7.834078	11.219076	0.932626
H	8.115163	11.018659	-0.810565
H	13.320740	-0.602099	6.332266
H	13.538747	-2.012314	5.282539
H	12.579965	-2.157395	6.772511
C	-8.279272	10.567081	0.150771
C	-12.814626	-1.490847	5.930137
H	-9.377007	-10.561799	-0.354700
H	-7.836204	-11.218854	-0.931314
H	-8.114737	-11.019169	0.812384
H	-13.321036	0.601530	-6.331056
H	-13.538355	2.012514	-5.282224
H	-12.579693	2.156245	-6.772402
H	-8.899354	10.687448	-0.751136
H	-7.474381	11.316910	0.092293
H	-8.901088	10.810189	1.023295
H	-13.321551	-0.599725	6.332322
H	-13.539003	-2.010695	5.283495
H	-12.580506	-2.154563	6.773762

Table S11. The coordinate of modified *p*CNQ-TPA in S_0 state

	Coordinates /Å		
Elements	**X**	**Y**	**Z**
C	1.215589	-0.694760	-0.154124
C	-0.000244	-1.388922	-0.283334
C	1.215664	0.694411	0.155622
C	-1.216003	-0.694689	-0.153853
C	-0.000315	-2.793538	-0.563047
N	2.388647	-1.331359	-0.416424
C	-0.000101	1.388646	0.285087
N	2.388821	1.330952	0.417614
C	-1.215934	0.694482	0.155899
N	-2.389157	-1.331207	-0.415927
N	-0.000367	-3.935290	-0.752046

C	3.504911	-0.672908	-0.292460
C	-0.000034	2.793291	0.564647
C	3.505021	0.672445	0.293356
N	-2.388994	1.331094	0.418144
C	-3.505350	-0.672687	-0.291721
N	4.669703	-1.291983	-0.728213
N	0.000007	3.935076	0.753454
N	4.669958	1.291452	0.728816
C	-3.505268	0.672655	0.294136
N	-4.670254	-1.291633	-0.727365
C	4.957594	-2.668281	-0.585459
C	5.729695	-0.696771	-1.444911
C	4.957887	2.667737	0.586012
C	5.730136	0.696157	1.445172
N	-4.670068	1.291761	0.729781
C	-4.958254	-2.667914	-0.584698
C	-5.730264	-0.696262	-1.443892
C	4.215602	-3.686367	0.008861
C	6.231196	-2.919145	-1.123957
C	5.851511	0.585434	-1.973676
C	6.718309	-1.667987	-1.679275
C	4.215777	3.685884	-0.008056
C	6.231669	2.918509	1.124131
C	5.852037	-0.586074	1.973855
C	6.718877	1.667306	1.679262
C	-4.957878	2.668083	0.587002
C	-5.730317	0.696550	1.446122
C	-4.216289	-3.686115	0.009459
C	-6.231935	-2.918618	-1.123082
C	-5.852018	0.586010	-1.972508
C	-6.718992	-1.667367	-1.678240
C	4.785462	-4.952045	0.065539
H	3.206897	-3.516485	0.375576
C	6.781187	-4.196399	-1.056511
C	7.007535	0.892522	-2.679440
H	5.079773	1.342844	-1.853646
C	7.868651	-1.339603	-2.390906
C	4.785700	4.951528	-0.064878
H	3.206949	3.516073	-0.374462
C	6.781717	4.195731	1.056551
C	7.008261	-0.893253	2.679252
H	5.080215	-1.343432	1.854040
C	7.869419	1.338831	2.390529
C	-4.215755	3.686128	-0.007203

C	-6.231711	2.918926	1.124987
C	-5.852286	-0.585632	1.974903
C	-6.719025	1.667755	1.680109
C	-4.786256	-4.951745	0.066093
H	-3.207530	-3.516352	0.376082
C	-6.782036	-4.195827	-1.055681
C	-7.008083	0.893266	-2.678133
H	-5.080202	1.343339	-1.852460
C	-7.869378	-1.338807	-2.389719
C	6.063045	-5.231578	-0.455310
H	4.201323	-5.765655	0.497336
H	7.780857	-4.381272	-1.452436
C	8.033731	-0.046612	-2.890825
H	7.126531	1.904635	-3.067722
H	8.623191	-2.102482	-2.588198
C	6.063457	5.230968	0.455591
H	4.201482	5.765186	-0.496476
H	7.781517	4.380533	1.452179
C	8.034577	0.045813	2.890351
H	7.127316	-1.905385	3.067464
H	8.624065	2.101660	2.587615
C	-4.785695	4.951765	-0.064242
H	-3.206973	3.516226	-0.373693
C	-6.781804	4.196104	1.057117
C	-7.008561	-0.892717	2.680259
H	-5.080476	-1.343021	1.855205
C	-7.869611	1.339386	2.391351
C	-6.063922	-5.231119	-0.454641
H	-4.202147	-5.765444	0.497762
H	-7.781766	-4.380578	-1.451510
C	-8.034382	-0.045754	-2.889504
H	-7.127034	1.905426	-3.066307
H	-8.624018	-2.101592	-2.586997
C	6.628566	-6.602452	-0.373862
C	9.256430	0.324917	-3.647557
C	6.629039	6.601809	0.374004
C	9.257491	-0.325815	3.646689
C	-6.063358	5.231338	0.456386
H	-4.201370	5.765198	-0.496148
H	-7.781711	4.381118	1.452354
C	-8.034851	0.046403	2.891243
H	-7.127670	-1.904815	3.068544
H	-8.624207	2.102278	2.588375
C	-6.629562	-6.601948	-0.373238

C	-9.257122	0.325958	-3.646081
C	6.453932	-7.391208	0.767127
C	7.358876	-7.149223	-1.437145
C	9.191008	1.146686	-4.776585
C	10.517802	-0.140813	-3.253704
C	6.454149	7.390584	-0.766935
C	7.359674	7.148524	1.437091
C	9.192373	-1.147626	4.775704
C	10.518768	0.139853	3.252456
C	-6.628495	6.602407	0.375546
C	-9.257808	-0.325120	3.647562
C	-6.454880	-7.390806	0.767672
C	-7.360031	-7.148571	-1.436489
C	-9.191716	1.147709	-4.775123
C	-10.518513	-0.139580	-3.252065
C	6.988193	-8.674053	0.842001
H	5.909379	-6.987681	1.622685
C	7.891143	-8.429169	-1.357616
H	7.491897	-6.569105	-2.352134
C	10.340260	1.488684	-5.483073
H	8.221874	1.508123	-5.125071
C	11.661528	0.201848	-3.962534
H	10.605438	-0.764270	-2.361967
C	6.988476	8.673393	-0.841946
H	5.909350	6.987089	-1.622351
C	7.892004	8.428437	1.357426
H	7.492914	6.568386	2.352035
C	10.341827	-1.489723	5.481816
H	8.223329	-1.509025	5.124477
C	11.662696	-0.202907	3.960912
H	10.606162	0.763333	2.360711
C	-7.357141	7.149455	1.435824
C	-6.452136	7.391924	-0.768378
C	-9.192776	-1.146923	4.776588
C	-10.519038	0.140661	3.253313
C	-6.989252	-8.673608	0.842503
H	-5.910195	-6.987397	1.623201
C	-7.892407	-8.428473	-1.357002
H	-7.493088	-6.568372	-2.351421
C	-10.341007	1.489874	-5.481470
H	-8.222567	1.508988	-5.123733
C	-11.662277	0.203251	-3.960751
H	-10.606127	-0.763018	-2.360313
C	7.715814	-9.218233	-0.216593

H	6.841205	-9.262775	1.750483
H	8.449665	-8.830156	-2.207125
C	11.596110	1.024110	-5.091694
H	10.255606	2.126544	-6.365945
H	12.631880	-0.171487	-3.625641
C	7.716412	9.217522	0.216460
H	6.841295	9.262125	-1.750390
H	8.450792	8.829376	2.206781
C	11.597581	-1.025205	5.090063
H	10.257412	-2.127620	6.364684
H	12.632966	0.170373	3.623722
C	-7.889609	8.432718	1.354727
H	-7.491318	6.571271	2.351827
C	-6.984126	8.672146	-0.844452
H	-5.906891	6.986398	-1.622592
C	-10.342268	-1.488906	5.482693
H	-8.223767	-1.508391	5.125388
C	-11.663003	-0.201985	3.961762
H	-10.606367	0.764163	2.361577
C	-7.717037	-9.217638	-0.216054
H	-6.842217	-9.262416	1.750921
H	-8.451048	-8.829347	-2.206485
C	-11.596877	1.025492	-5.089928
H	-10.256370	2.127704	-6.364366
H	-12.632643	-0.169931	-3.623729
C	8.288351	-10.608758	-0.146350
C	12.843556	1.391047	-5.850365
C	8.288955	10.608038	0.146093
C	12.845237	-1.392198	5.848362
C	-7.713618	9.218914	0.215860
H	-8.448064	8.834965	2.203171
H	-6.836007	9.260019	-1.753779
C	-11.597976	-1.024281	5.090919
H	-10.257918	-2.126786	6.365579
H	-12.633231	0.171404	3.624574
C	-8.289747	-10.608093	-0.145839
C	-12.844364	1.392589	-5.848455
H	9.368946	-10.607754	-0.357253
H	7.814476	-11.271732	-0.887703
H	8.138090	-11.055678	0.846081
H	13.364347	0.493976	-6.220292
H	13.554047	1.936249	-5.209234
H	12.614893	2.028303	-6.715664
H	9.369434	10.607133	0.357571

H	7.814662	11.271225	0.886993
H	8.139194	11.054658	-0.846548
H	13.365795	-0.495175	6.218739
H	13.555816	-1.936810	5.206832
H	12.616878	-2.030009	6.713333
C	-8.279567	10.610896	0.124201
C	-12.845679	-1.391196	5.849178
H	-9.370487	-10.606847	-0.356006
H	-7.816489	-11.270923	-0.887713
H	-8.138895	-11.055330	0.846358
H	-13.365214	0.495591	-6.218476
H	-13.554790	1.937722	-5.207196
H	-12.615737	2.029956	-6.713684
H	-8.925223	10.722103	-0.760780
H	-7.478216	11.361644	0.036522
H	-8.877259	10.861084	1.011529
H	-13.366612	-0.494112	6.218868
H	-13.555936	-1.936450	5.207832
H	-12.617304	-2.028397	6.714594

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