

Why orientation of azulene affects two-photon activity in a porphyrinoid-azulene system?

ELECTRONIC SUPPLEMENTARY INFORMATION

Swati Singh Rajput,^a Nikita Raghuvanshi,^b Tejendra Banana,^a Pooja Yadav,^a and Md. Mehboob Alam,^{a*}

^aDepartment of Chemistry, Indian Institute of Technology, Bhilai, Chhattisgarh, 491001, India.

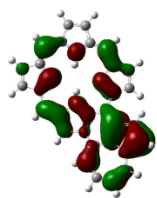
^bCentre for Basic Sciences, Pt. Ravishankar Shukla University, Raipur, Chhattisgarh, 492010, India
E-mail: mehboob@iitbhilai.ac.in

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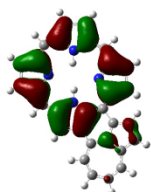
1. Orbital diagrams.
2. Absorption wavelength and orbital contribution.
3. Natural transition orbital plots.
4. Cartesian coordinates of ground state optimized geometry of all the systems[B3LYP/6-311+G(d,p)].
5. Magnitudes of different transition dipole moment vector.
6. Two-photon absorption cross section.

1. Orbital diagram:-

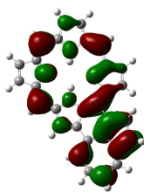
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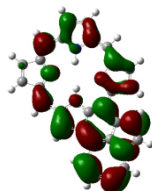
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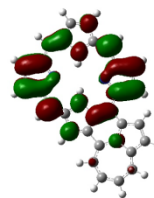
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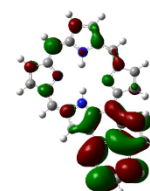
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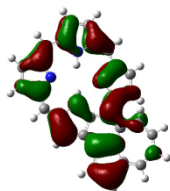


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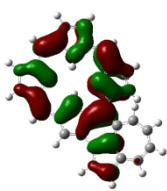


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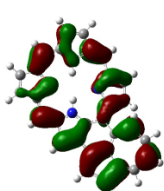
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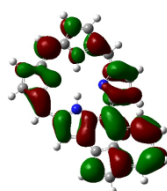
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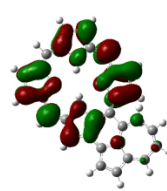
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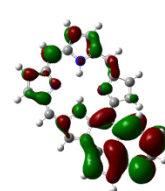
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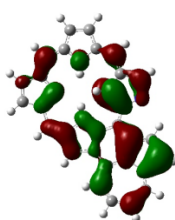


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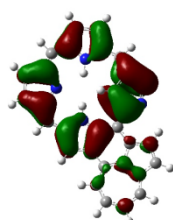


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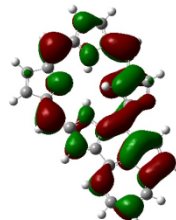
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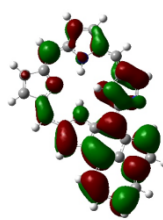
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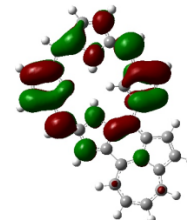
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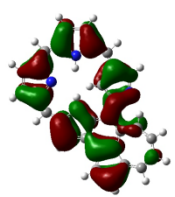


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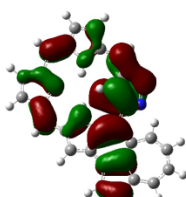


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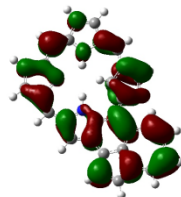
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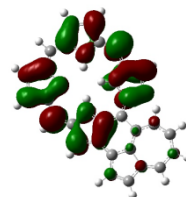
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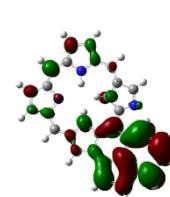
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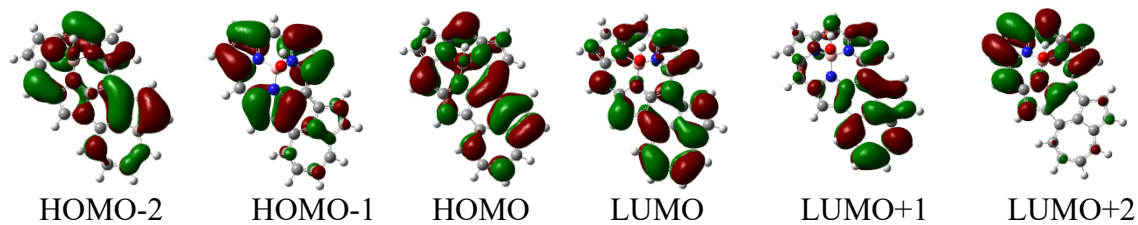


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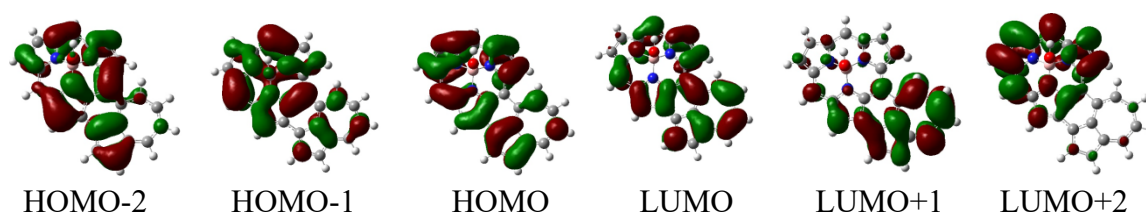


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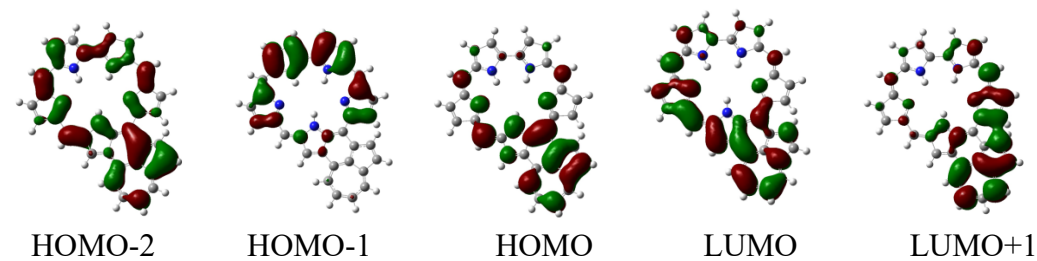
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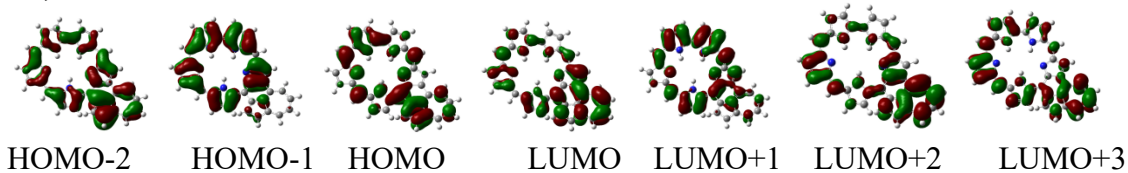
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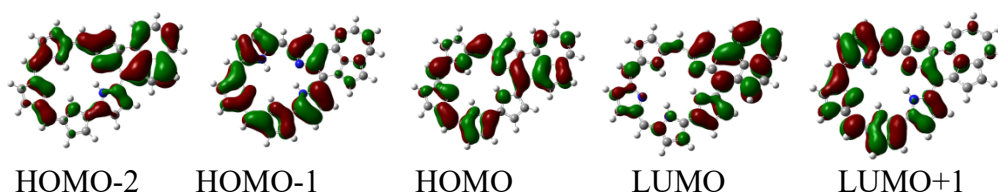
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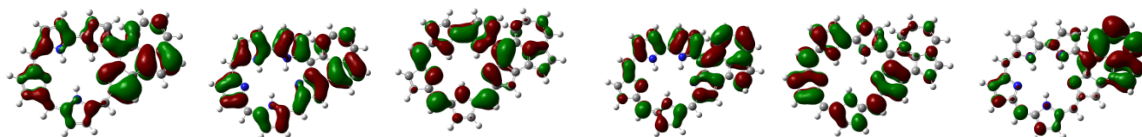
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S-4,5-HP:-



S-4,5-PH:-



HOMO-2

HOMO-1

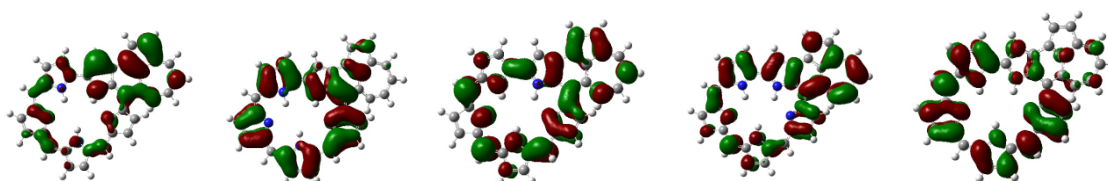
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LUMO

LUMO+1

LUMO+2

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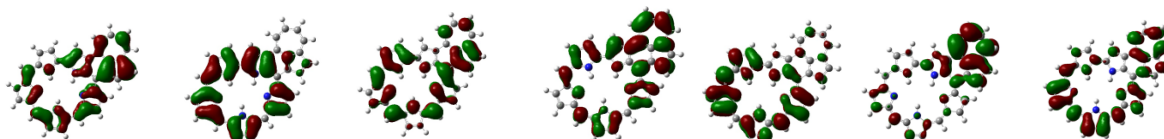
HOMO-1

HOMO

LUMO

LUMO+1

S-5,6-PH:-



HOMO-2

HOMO-1

HOMO

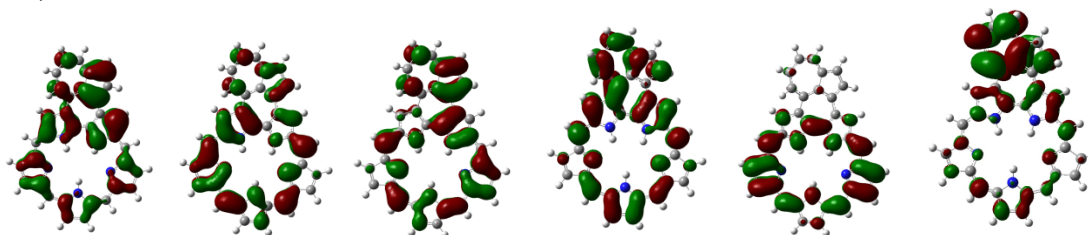
LUMO

LUMO+1

LUMO+2

LUMO+3

S-7,7-HP:-



HOMO-2

HOMO-1

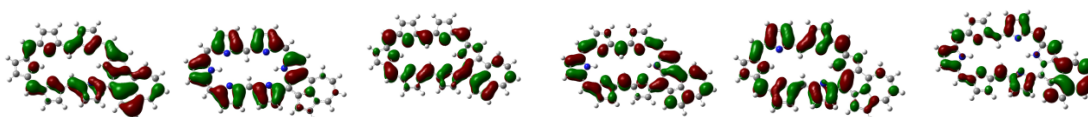
HOMO

LUMO

LUMO+1

LUMO+2

Hx-1,2-HP:-



HOMO-2

HOMO-1

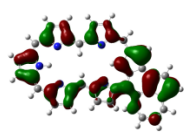
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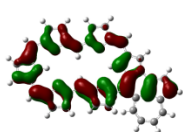
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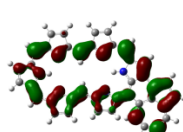
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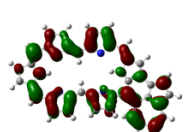
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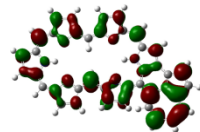
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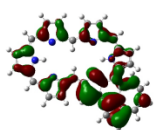


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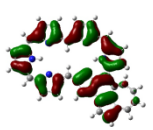


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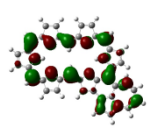
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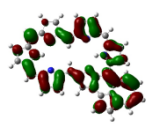
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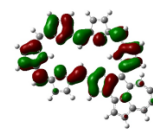
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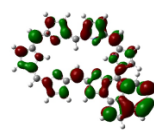
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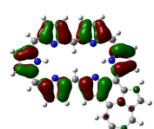


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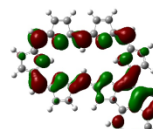


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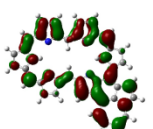
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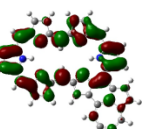
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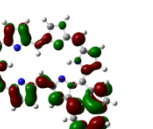
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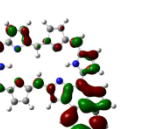
LUMO



LUMO+1

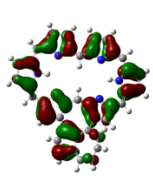


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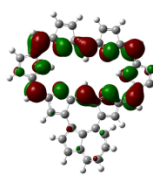


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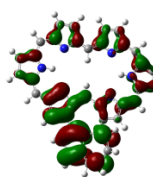
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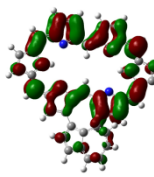
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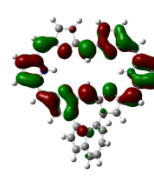
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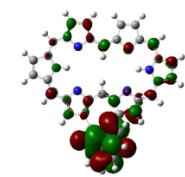
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LUMO



LUMO+1



LUMO+2

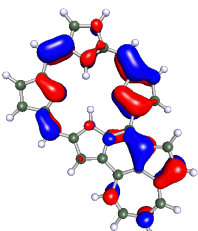
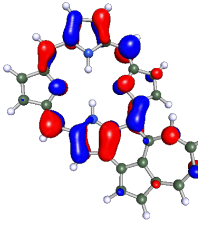
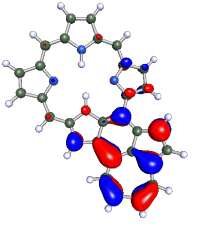
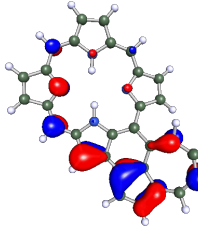
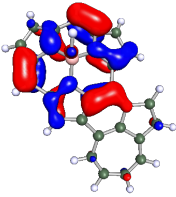
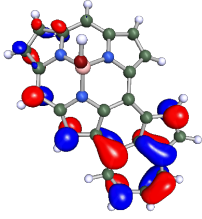
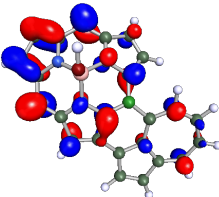
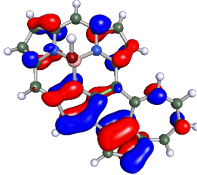
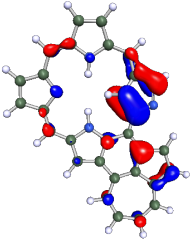
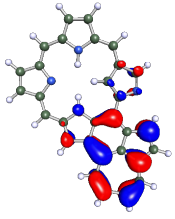
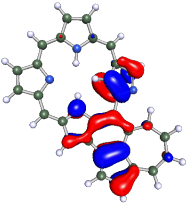
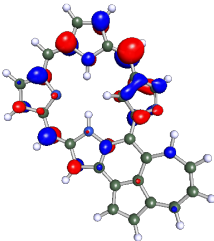
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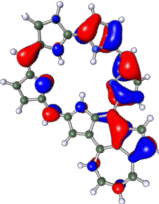
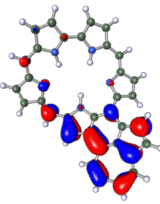
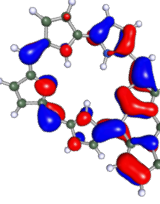
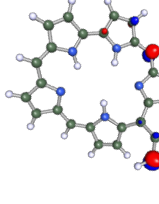
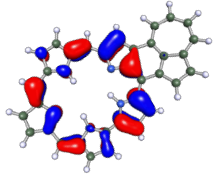
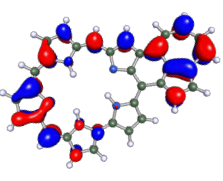
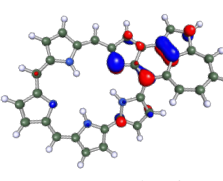
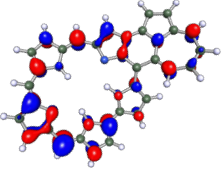
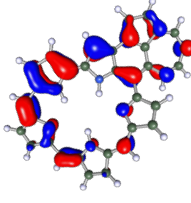
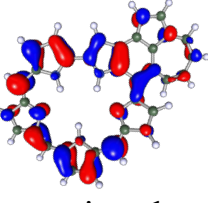
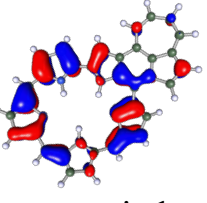
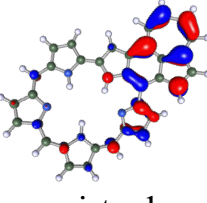
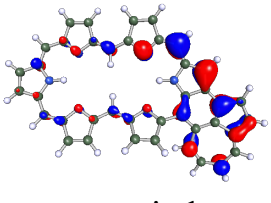
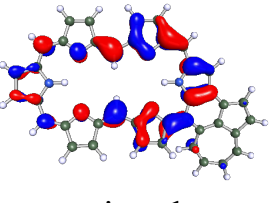
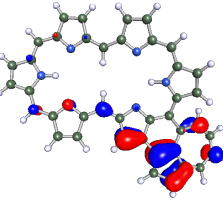
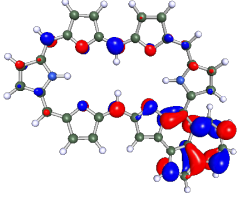
System	Excited state	Absorption spectra(nm)	Transition	Orbital contribution	Percentage contribution
Pr-1,2-HP	5	432	S ₀ ->S ₅	HOMO-2 -> LUMO HOMO-1 -> LUMO HOMO -> LUMO+1	30.6% 13.5% 12.2%
Pr-1,2-PH	5	422	S ₀ ->S ₅	HOMO-1 -> LUMO HOMO -> LUMO+1	33.4% 25.6%
NCP-1,2-HP	5	447	S ₀ ->S ₅	HOMO-2 -> LUMO HOMO-1 -> LUMO	25.2% 24.0%
NCP-1,2-PH	5	441	S ₀ ->S ₅	HOMO-2 -> LUMO+1 HOMO-1 -> LUMO+1 HOMO -> LUMO+1	31.7% 19.2% 14.7%
SP-1,2-HP	5	387	S ₀ ->S ₅	HOMO-2 -> LUMO HOMO-1 -> LUMO+1	35.1% 26.0%
SP-1,2-PH	5	393	S ₀ ->S ₅	HOMO -> LUMO+1	47.1%
S-1,2-HP	5	472	S ₀ ->S ₅	HOMO-2 -> LUMO HOMO-1 -> LUMO HOMO -> LUMO+1	37.8% 15.9% 14.2%
S-2,3-PH	5	468	S ₀ ->S ₅	HOMO-1 -> LUMO+1 HOMO -> LUMO+3 HOMO-1 -> LUMO HOMO -> LUMO+1	26.1% 18.8% 12.0% 10.7%
S-4,5-HP	5	474	S ₀ ->S ₅	HOMO-1 -> LUMO+1 HOMO-2 -> LUMO	34.7% 16.2%
S-4,5-PH	5	465	S ₀ ->S ₅	HOMO-1 -> LUMO+1 HOMO-2 -> LUMO+1	23.0% 21.1%
S-5,6-HP	5	472	S ₀ ->S ₅	HOMO-1 -> LUMO HOMO -> LUMO+1	29.9% 29.7%
S-5,6-PH	5	540	S ₀ ->S ₅	HOMO -> LUMO+1 HOMO-2 -> LUMO	37.2% 18.3%
S-7,7-PH	5	454	S ₀ ->S ₅	HOMO -> LUMO+1 HOMO-1 -> LUMO+2	25.0% 19.8%
Hx-1,2-HP	5	531	S ₀ ->S ₅	HOMO-1 -> LUMO HOMO -> LUMO+2 HOMO-1 -> LUMO+1 HOMO -> LUMO+1	32.6% 16.2% 14.7% 14.0%
Hx-1,2-PH	5	531	S ₀ ->S ₅	HOMO-1 -> LUMO HOMO -> LUMO+2 HOMO-1 -> LUMO+1 HOMO -> LUMO+1	32.6% 16.2% 14.7% 14.0%
Hx-2,3-HP	5	532	S ₀ ->S ₅	HOMO -> LUMO+2 HOMO-2 -> LUMO HOMO -> LUMO+1	20.9% 14.6% 14.4%
Hx-2,3-PH	5	520	S ₀ ->S ₅	HOMO-1 -> LUMO+1 HOMO -> LUMO+3 HOMO-1 -> LUMO	27.0% 15.6% 10.7%

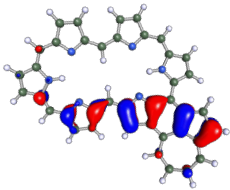
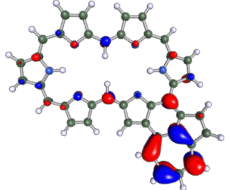
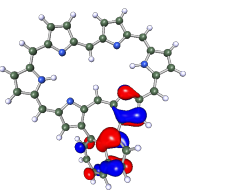
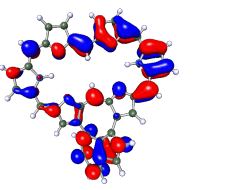
Hx-4,4-HP	5	568	$S_0 \rightarrow S_5$	HOMO-2 \rightarrow LUMO+1 HOMO-2 \rightarrow LUMO+2 HOMO-2 \rightarrow LUMO	30.3% 17.3% 11.7%
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Table S1: Different selected excited state, absorption spectra, transition, orbital contribution and percentage contribution involved for porphyrinoid-azulene systems.

3. Natural transition orbital:- This includes the natural transition orbital plots for all the system considered in this work, that are calculated at RICC2/cc-pVDZ level of theory and plotted utilizing Turbomole 7.3 package.

Pr-1,2-HP NTOs		Pr-1,2-PH NTOs	
 occupied	 virtual	 occupied	 virtual
SP-1,2-HP NTOs		SP-1,2-PH NTOs	
 occupied	 virtual	 occupied	 virtual
NCP-1,2-HP NTOs		NCP-1,2-PH NTOs	
 occupied	 virtual	 occupied	 virtual
S-1,2-HP NTOs		S-2,3-PH NTOs	

 occupied	 virtual	 occupied	 virtual
S-4,5-HP NTOs		S-4,5-PH NTOs	
 occupied	 virtual	 occupied	 virtual
S-5,6-HP NTOs		S-5,6-PH NTOs	
 occupied	 virtual	 occupied	 virtual
S-7,7-HP NTOs		Hx-1,2-HP NTOs	
 occupied	 virtual	 occupied	 virtual
Hx-1,2-PH NTOs		Hx-2,3-HP NTOs	

Hx-2,3-PH NTO		Hx-4,4-HP NTOs	
			
occupied	virtual	occupied	virtual

4. Cartesian coordinates:- This includes the optimized cartesian coordinates for all the system considered in this work, that are optimized at B3LYP/6-311+G(d,p) level of theory using Gaussian 16 program.

Pr-1,2-HP			
N	3.808971	-0.919508	0.074267
N	0.882822	-1.745046	-0.039317
N	0.081203	0.978866	-0.071275
N	2.945019	1.807670	0.048721
C	5.042541	-0.328055	0.171255
C	6.007341	-1.390841	0.170149
C	5.330054	-2.575186	0.053375
C	3.925590	-2.283683	-0.011500
C	2.884457	-3.190332	-0.159126
C	1.505434	-2.944654	-0.207849
C	0.535120	-3.997175	-0.453022
C	-0.686321	-3.408081	-0.415946
C	-0.454811	-1.998219	-0.130576
C	-1.454345	-0.995231	-0.000215
C	-1.143803	0.382504	-0.041157
C	-2.125349	1.423623	-0.111999
C	-1.437036	2.629854	-0.178639
C	-0.049429	2.348330	-0.136328
C	0.994935	3.283452	-0.120887
C	2.359489	3.039939	-0.024157
C	3.367959	4.094232	0.028578
C	4.564811	3.469638	0.139132
C	4.279354	2.037667	0.144839
C	5.265371	1.043326	0.216877
H	7.074808	-1.246038	0.238967
H	5.746493	-3.570371	0.012593
H	3.185912	-4.227586	-0.255999
H	0.767932	-5.032730	-0.656928
H	-1.633942	-3.874592	-0.623621
H	-1.845274	3.626755	-0.239855
H	0.685993	4.321556	-0.171843

H	3.167750	5.155545	-0.012000
H	5.547977	3.913392	0.206472
H	6.297422	1.365337	0.289867
H	2.944815	-0.390975	0.044185
H	0.954647	0.467445	-0.016966
C	-3.548233	1.117311	-0.102148
C	-4.478168	2.169964	-0.217851
C	-3.855982	-0.245131	0.048721
C	-5.867981	2.134169	-0.195871
H	-4.050123	3.158041	-0.345441
C	-5.178713	-0.876766	0.246018
C	-2.877216	-1.261163	0.144292
C	-6.744295	1.060983	-0.013321
H	-6.348827	3.099628	-0.328143
C	-6.431619	-0.281508	0.203408
C	-4.935104	-2.247914	0.502166
C	-3.568481	-2.473213	0.459012
H	-7.800985	1.308177	-0.024693
H	-7.274915	-0.950359	0.357537
H	-5.697191	-2.984167	0.714771
H	-3.101996	-3.419983	0.680957

Pr-1,2-PH			
N	3.601109	-1.226614	0.091786
N	0.602775	-1.622154	-0.092674
N	0.197608	1.196779	-0.101658
N	3.126593	1.599489	0.113046
C	4.898366	-0.820121	0.266229
C	5.705232	-1.999170	0.239144
C	4.874700	-3.072980	0.020413
C	3.534981	-2.584194	-0.076793
C	2.377119	-3.322604	-0.335670
C	1.058488	-2.882455	-0.395275
C	-0.044002	-3.740550	-0.787266
C	-1.166754	-2.983876	-0.703036
C	-0.740996	-1.666253	-0.230226
C	-1.596683	-0.531612	-0.023866
C	-1.097972	0.777429	-0.083522
C	-1.930796	1.952575	-0.211021
C	-1.088093	3.045162	-0.291281
C	0.254626	2.574006	-0.195479
C	1.414580	3.339626	-0.145376
C	2.732799	2.894440	0.020605
C	3.875506	3.796276	0.136888
C	4.964968	3.008899	0.308982
C	4.481496	1.633260	0.282278
C	5.305113	0.512113	0.375212
H	6.778329	-2.010021	0.354864
H	5.153209	-4.112092	-0.068655

H	2.537800	-4.378672	-0.523866
H	0.043626	-4.765404	-1.118853
H	-2.166457	-3.267694	-0.988435
H	-1.362177	4.083750	-0.395004
H	1.269198	4.411784	-0.214581
H	3.829393	4.875183	0.094009
H	5.995582	3.309376	0.433504
H	6.367760	0.681548	0.505009
H	2.819489	-0.582262	0.054989
H	0.996028	0.581874	-0.003817
C	-3.343784	1.761220	-0.243048
C	-3.867355	0.482397	-0.008272
C	-4.428564	2.675715	-0.405752
C	-3.054297	-0.661063	0.192276
C	-5.339539	0.620455	-0.003528
H	-4.326915	3.738035	-0.584050
C	-5.622271	1.989148	-0.285861
C	-3.556963	-1.877346	0.704211
C	-6.297282	-0.347355	0.246865
H	-6.615957	2.407265	-0.361858
C	-4.871466	-2.306520	0.888839
H	-2.809317	-2.592642	1.017495
C	-6.087471	-1.668754	0.649327
H	-7.332626	-0.026456	0.162769
H	-4.957491	-3.315149	1.284606
H	-6.978173	-2.258148	0.842397

NCP-1,2-HP			
H	7.140660	-1.177525	0.180130
H	5.875595	-3.542344	0.210326
H	3.276449	-4.286489	-0.017956
H	0.669137	-4.885697	-0.671312
H	-1.968476	3.656876	-0.012839
H	0.657103	4.381934	-0.136917
H	3.116046	5.151579	-0.198245
H	6.260340	1.431601	0.023793
H	3.017021	-0.418480	-0.033166
H	0.944149	0.651610	-0.146445
C	5.082397	-0.317513	0.096462
C	6.075710	-1.351796	0.158034
C	5.427958	-2.560627	0.169375

C	4.014223	-2.322061	0.125677
C	2.978834	-3.246294	0.069550
C	1.606464	-2.946559	0.043610
C	0.539088	-3.850969	-0.371892
C	-0.416236	-1.935284	-0.008382
C	-1.459469	-0.971756	0.005013
C	-1.182651	0.419721	0.018586
C	-2.184116	1.438809	0.037961
C	-1.528901	2.671675	-0.005269
C	-0.139124	2.423439	-0.055372
C	0.932172	3.333912	-0.107525
C	2.292196	3.047038	-0.110548
C	3.312737	4.089939	-0.150903
C	4.222315	2.028379	-0.048039
C	5.241035	1.064348	0.024586
N	3.868011	-0.947386	0.099065
N	0.025677	1.059337	-0.040085
N	2.878418	1.803124	-0.054295
N	-0.630550	-3.272668	-0.406663
C	0.942506	-1.732149	0.290991
H	1.359066	-0.882072	0.802421
C	4.508478	3.459735	-0.112342
H	5.496725	3.897047	-0.121183
C	-3.599654	1.090242	0.057151
C	-4.558082	2.119430	0.110146
C	-3.870569	-0.289208	0.010952
C	-5.947794	2.040409	0.124710
H	-4.159620	3.127367	0.146405
C	-5.175490	-0.983663	0.010732
C	-2.869172	-1.282878	-0.024633
C	-6.790595	0.927865	0.094659
H	-6.456789	2.999371	0.167344
C	-6.443767	-0.424562	0.046071
C	-4.894881	-2.375678	-0.027151
C	-3.524361	-2.557658	-0.041639
H	-7.854130	1.143887	0.115236
H	-7.270683	-1.130268	0.035842
H	-5.643894	-3.154838	-0.039520
H	-2.997117	-3.498151	-0.073486

NCP-1,2-PH			
H	6.892826	-1.905418	0.326787
H	5.317120	-4.074772	0.138355
H	2.658456	-4.422677	-0.323679
H	0.078829	-4.578589	-1.177577
H	-1.481858	4.094982	-0.161778
H	1.205917	4.431926	-0.205418
H	3.731803	4.893098	-0.124729
H	6.380930	0.810141	0.262628

H	2.926142	-0.577568	-0.009935
H	0.979042	0.682999	-0.148846
H	-4.410483	3.739553	-0.120397
H	-6.688203	2.373686	-0.035600
H	-2.864846	-2.797379	0.376860
H	-7.386478	-0.099202	0.125137
H	-5.009106	-3.551751	0.513903
H	-7.030712	-2.420319	0.361763
C	4.977994	-0.774255	0.212769
C	5.816544	-1.928970	0.250088
C	5.008439	-3.040293	0.148616
C	3.652431	-2.604045	0.065056
C	2.496034	-3.368704	-0.119098
C	1.186401	-2.893983	-0.140030
C	0.050120	-3.593916	-0.723294
C	-0.696136	-1.639195	-0.112938
C	-1.632559	-0.546812	-0.006272
C	-1.159402	0.772048	-0.025543
C	-2.005818	1.944876	-0.052372
C	-1.183768	3.058766	-0.122825
C	0.163716	2.605966	-0.134373
C	1.338896	3.357380	-0.156168
C	2.661037	2.899158	-0.085746
C	3.798942	3.816179	-0.064789
C	4.449704	1.664711	0.090565
C	5.323079	0.583522	0.200655
C	-3.412410	1.740137	-0.036291
C	-3.921578	0.436575	0.037100
C	-4.505529	2.662905	-0.071478
C	-3.100364	-0.721549	0.084956
C	-5.393685	0.563906	0.056882
C	-5.690134	1.959445	-0.025709
C	-3.608493	-2.020012	0.292439
C	-6.351364	-0.430576	0.147017
C	-4.924407	-2.478147	0.368918
C	-6.140148	-1.804021	0.287332
N	3.690550	-1.227002	0.129574
N	0.132727	1.228965	-0.086666
N	3.082142	1.605697	0.004201
N	-1.034845	-2.870252	-0.729935
C	0.649641	-1.639545	0.251893
H	1.138481	-0.917392	0.885160
C	4.907606	3.050054	0.048775
H	5.939403	3.367212	0.100339

SP-1,2-HP			
C	-2.039773	3.297638	-0.708843

C	-0.698759	3.144361	-0.422102
C	-2.720864	2.110885	-0.266831
C	-0.522924	1.871747	0.220946
N	-1.784344	1.341481	0.364984
C	-3.974146	1.550087	-0.609125
H	-4.703927	2.153521	-1.132279
C	-4.165430	0.162341	-0.492087
C	-5.046965	-0.778489	-1.147393
N	-3.212865	-0.586787	0.136806
C	-4.522260	-2.037318	-0.974442
C	-3.302018	-1.912076	-0.208235
C	-2.194235	-2.755776	-0.040349
H	-2.254093	-3.788698	-0.356580
C	-0.939380	-2.194272	0.312939
C	0.419441	-2.580580	0.076217
N	-0.908851	-0.874882	0.685369
C	1.216248	-1.434839	0.218684
C	0.327838	-0.366079	0.547560
C	0.597983	1.014769	0.410228
B	-2.104701	-0.012201	1.003136
O	-2.348956	0.008092	2.416805
H	-3.089898	0.566259	2.665728
H	0.730835	-3.559688	-0.255312
H	0.094227	3.817282	-0.708235
H	-2.493683	4.111995	-1.253522
H	-5.912466	-0.514892	-1.736815
H	-4.896025	-2.956091	-1.401489
C	2.623489	-1.123791	-0.008985
C	3.533144	-2.178753	-0.213300
C	2.944110	0.255285	0.014543
C	4.906225	-2.142218	-0.435380
H	3.100469	-3.173257	-0.182114
C	4.263735	0.902126	-0.158881
C	2.002250	1.295338	0.208866
C	5.783307	-1.058154	-0.517078
H	5.371006	-3.116406	-0.561250
C	5.492994	0.301290	-0.391654
C	4.054444	2.301256	-0.047977
C	2.705361	2.533457	0.173229
H	6.823824	-1.307236	-0.699320
H	6.336369	0.980530	-0.489992
H	4.831385	3.049234	-0.117457
H	2.256664	3.505638	0.325093

SP-1,2-PH

C	-1.414980	3.330834	-0.766437
C	-0.116031	2.934053	-0.518250
C	-2.287237	2.303760	-0.276826
C	-0.156831	1.661954	0.154190
N	-1.483528	1.376480	0.339696
C	-3.629144	1.983852	-0.570160
H	-4.247680	2.709552	-1.082147
C	-4.085294	0.661066	-0.419242
C	-5.138435	-0.097751	-1.043119
N	-3.263803	-0.251358	0.184412
C	-4.843731	-1.435196	-0.880827
C	-3.604137	-1.530876	-0.151423
C	-2.653965	-2.570231	-0.019010
H	-2.914733	-3.571055	-0.336802
C	-1.316372	-2.252862	0.277749
C	-0.050145	-2.893024	0.009064
N	-1.030736	-0.958810	0.640436
C	0.940548	-1.920868	0.114556
C	0.274172	-0.693446	0.466877
C	0.798274	0.606520	0.349795
B	-2.031061	0.107415	1.000776
O	-2.212676	0.175459	2.421840
H	-2.850056	0.841186	2.692226
H	0.067937	-3.915037	-0.317400
H	0.773525	3.439628	-0.857498
H	-1.725970	4.205516	-1.317952
H	-5.958346	0.318891	-1.608852
H	-5.389508	-2.270588	-1.293371
C	2.345180	-1.792058	-0.145440
C	2.953191	-0.520917	-0.072302
C	3.347877	-2.754167	-0.462738
C	2.259280	0.691434	0.193077
C	4.393606	-0.728478	-0.346436
H	3.174309	-3.816591	-0.572040
C	4.571016	-2.119668	-0.589189
C	2.875817	1.944415	0.372784
C	5.415214	0.206819	-0.371547
H	5.517688	-2.586773	-0.820796
C	4.211839	2.321563	0.238935
H	2.213728	2.741047	0.688580
C	5.337624	1.576684	-0.106803
H	6.402937	-0.180023	-0.610164
H	4.403443	3.372184	0.440474
H	6.271880	2.126654	-0.158326

S-1,2-HP

C	5.182967	1.487895	0.703541
C	6.406756	0.876315	1.087389

C	4.896923	-0.747192	0.623493
N	4.286190	0.469872	0.463826
H	3.353485	0.698747	0.122042
H	7.305046	1.411069	1.355212
C	4.308893	-1.995532	0.342806
C	4.970847	-3.243922	0.213432
C	4.046480	-4.173196	-0.216838
C	2.792101	-3.521925	-0.340088
N	2.992469	-2.203041	0.010446
H	4.220009	-5.215769	-0.435178
C	0.317993	-3.453208	-0.749449
C	-0.876427	-4.176565	-1.128034
C	-1.916671	-3.336583	-0.904433
H	-0.901519	-5.182742	-1.521641
H	-2.958964	-3.507474	-1.117188
C	1.567667	-4.063286	-0.726933
C	-1.341978	-2.095090	-0.401362
N	0.009097	-2.168047	-0.350305
C	-0.707812	2.327145	-0.648499
C	-1.794815	0.383091	-0.211713
H	-2.506658	3.591904	-0.708975
C	1.598479	3.515881	-0.602012
C	2.178431	4.855715	-0.684218
C	3.464491	4.744417	-0.280490
C	3.671716	3.337372	0.022118
N	2.530153	2.610185	-0.197383
H	1.645748	5.745683	-0.988114
H	4.210846	5.520539	-0.188729
C	-2.162198	-0.965232	-0.079746
C	-2.096571	2.602981	-0.576644
C	0.225658	3.357974	-0.808779
N	-0.565406	0.964261	-0.441912
C	4.887315	2.832336	0.483244
H	1.594550	-5.108102	-1.015775
H	5.689598	3.540551	0.652947
H	-0.269151	4.293180	-1.050422
H	2.208147	-1.563948	0.080116
H	0.300639	0.446965	-0.457668
C	6.232553	-0.491309	1.033062
H	6.023569	-3.403387	0.383985
H	6.965085	-1.249986	1.258603
C	-2.771506	1.438394	-0.264518
C	-3.554018	-1.159257	0.300250
C	-4.512624	-0.124745	0.284446
C	-4.202943	-2.321163	0.816855
C	-5.800481	-0.696612	0.741016
C	-4.188711	1.200020	-0.025643
C	-5.543843	-2.048763	1.062595
H	-3.715416	-3.262247	1.023975
C	-7.027662	-0.054820	0.844979

C	-5.095948	2.280569	-0.088310
H	-6.274464	-2.743422	1.452416
C	-7.330215	1.276959	0.563474
H	-7.855211	-0.672608	1.185580
C	-6.463410	2.297203	0.152554
H	-4.668674	3.239073	-0.360373
H	-8.367389	1.567713	0.695901
H	-6.935412	3.266453	0.015295

S-2,3-PH			
C	-5.499541	0.279536	0.790872
C	-6.333361	1.400334	1.044393
C	-4.307635	2.142702	0.355035
N	-4.274918	0.771911	0.399415
H	-3.552432	0.118910	0.095291
H	-7.356642	1.343637	1.382412
C	-3.232071	2.972649	-0.013805
C	-3.265000	4.375819	-0.234780
C	-1.994510	4.782815	-0.577801
C	-1.145907	3.642748	-0.560806
N	-1.942803	2.561144	-0.238076
H	-1.668997	5.785122	-0.810773
C	1.084267	2.493567	-0.560907
C	2.507827	2.654870	-0.524784
C	3.035123	1.421178	-0.238356
H	3.024882	3.591629	-0.672564
C	0.232956	3.591797	-0.715358
C	1.884060	0.514323	-0.167966
N	0.722267	1.178109	-0.350596
C	-0.684091	-3.111176	-0.805448
C	1.208854	-1.915633	-0.400115
H	0.369457	-4.898931	-1.588947
C	-3.236693	-3.194154	-0.374038
C	-4.332980	-4.155831	-0.275539
C	-5.389770	-3.484370	0.237384
C	-4.950746	-2.108354	0.403734
N	-3.635034	-1.962318	0.035053
H	-4.270104	-5.200041	-0.547163
H	-6.378192	-3.857440	0.464710
C	2.118099	-0.888130	-0.054673
C	0.443823	-3.905296	-1.174043
C	-1.976787	-3.633023	-0.799967
N	-0.175600	-1.892377	-0.390257
C	-5.803660	-1.083603	0.804258
H	0.713158	4.543131	-0.915185
H	-6.813925	-1.354275	1.087220

H	-1.983447	-4.664701	-1.136707
H	-1.534450	1.642093	-0.107338
H	-0.724426	-1.112724	-0.062272
C	-5.605812	2.540854	0.767570
H	-4.147504	4.990428	-0.156312
H	-5.938817	3.562514	0.859482
C	1.582368	-3.195283	-0.912110
H	2.595627	-3.494702	-1.116920
C	3.477360	-1.258187	0.310235
C	4.563751	-0.359125	0.281523
C	3.974947	-2.495854	0.822467
C	5.766332	-1.090817	0.723912
C	4.408528	0.999809	-0.027493
C	5.340642	-2.400730	1.053414
H	3.371708	-3.365119	1.040177
C	7.070171	-0.618247	0.814087
C	5.451380	1.947694	-0.106147
H	5.979548	-3.182461	1.439435
C	7.542101	0.660696	0.524941
H	7.811923	-1.340015	1.147593
C	6.812410	1.784564	0.118721
H	5.150162	2.953228	-0.377627
H	8.610048	0.812879	0.644876
H	7.406425	2.682714	-0.028621

S-4,5-HP			
C	-4.289764	-2.781126	-0.070518
C	-4.083338	-4.172640	-0.230068
C	-2.724934	-4.390839	-0.340010
C	-2.067495	-3.138094	-0.244366
N	-3.044621	-2.186052	-0.087856
H	-2.961564	-1.177750	-0.003060
H	-4.869528	-4.911420	-0.254763
H	-2.229680	-5.340253	-0.462766
C	-0.666738	-2.942113	-0.262805
C	0.299261	-3.962134	-0.442758
C	1.550001	-3.389747	-0.346761
C	1.384662	-2.003812	-0.100726
N	0.020848	-1.771591	-0.073491
H	0.078676	-4.999004	-0.637475
H	2.488386	-3.893904	-0.492822
C	1.993367	0.401239	-0.053782
C	3.027432	1.417433	-0.154522
C	2.352084	2.606357	-0.290524
H	2.756388	3.602114	-0.399322
C	2.344638	-0.971073	0.036005
C	0.950078	2.296472	-0.242217

N	0.747741	0.949335	-0.112260
C	-3.587825	3.236687	0.089767
C	-1.346507	3.510850	-0.180596
C	-1.971069	4.804257	-0.178329
H	-4.070875	5.406439	0.049189
H	-1.426211	5.729768	-0.287431
C	-5.376881	1.415595	0.287664
C	-6.815410	1.200661	0.425419
C	-7.008379	-0.136917	0.373637
C	-5.689752	-0.729204	0.209487
N	-4.713617	0.239378	0.169859
H	-7.553455	1.982333	0.536253
H	-7.936790	-0.686712	0.434165
C	0.023645	3.359424	-0.288240
C	-3.311525	4.641384	-0.005283
C	-4.865158	2.721930	0.249926
N	-2.371828	2.590085	-0.022079
C	-5.498629	-2.097907	0.087193
H	-6.386516	-2.719444	0.110490
H	-5.620839	3.495368	0.335442
H	0.513660	4.321162	-0.402652
H	-0.322873	-0.814390	0.005548
H	-2.261474	1.588867	0.013627
C	4.444465	1.109682	-0.102714
C	5.386465	2.149388	-0.240288
C	4.748275	-0.246600	0.112209
C	6.774629	2.104085	-0.182761
H	4.968954	3.134276	-0.417782
C	6.054341	-0.880338	0.359218
C	3.756368	-1.245709	0.222582
C	7.639581	1.033029	0.063465
H	7.266508	3.060049	-0.341314
C	7.314777	-0.297712	0.322823
C	5.792811	-2.243066	0.656574
C	4.426567	-2.456799	0.589063
H	8.697750	1.274599	0.067568
H	8.149491	-0.966008	0.519651
H	6.543551	-2.977787	0.910795
H	3.946503	-3.392238	0.830878

S-4,5-PH			
C	-3.937516	-3.013868	-0.227217
C	-3.588283	-4.358775	-0.520713
C	-2.221679	-4.421571	-0.667570
C	-1.692942	-3.116060	-0.459928
N	-2.758791	-2.291284	-0.210548
H	-2.777909	-1.292896	-0.026735
H	-4.294037	-5.171081	-0.603347
H	-1.632169	-5.297448	-0.884437

C	-0.324537	-2.776302	-0.453234
C	0.747320	-3.668064	-0.689523
C	1.928742	-2.977125	-0.512801
C	1.609323	-1.639762	-0.156610
N	0.234145	-1.555290	-0.146125
H	0.644215	-4.703521	-0.971145
H	2.920855	-3.361368	-0.674014
C	1.949313	0.807437	-0.127808
C	2.874258	1.923825	-0.346884
C	2.082474	3.017195	-0.553021
H	2.384449	4.035015	-0.751886
C	2.448913	-0.505250	0.036392
C	0.715420	2.567365	-0.413450
N	0.651973	1.215070	-0.182513
C	-3.844490	3.004671	0.264802
C	-1.687028	3.519533	-0.222350
C	-2.443431	4.735872	-0.158036
H	-4.563592	5.105798	0.289565
H	-2.016966	5.714265	-0.318468
C	-5.417229	0.999612	0.525058
C	-6.810798	0.628100	0.732978
C	-6.874613	-0.716415	0.577175
C	-5.520037	-1.152302	0.288597
N	-4.649395	-0.093455	0.275711
H	-7.614157	1.317576	0.950176
H	-7.739207	-1.361336	0.643051
C	-0.314858	3.516087	-0.449313
C	-3.734703	4.427642	0.155153
C	-5.040139	2.350243	0.520703
N	-2.578377	2.495534	0.031198
C	-5.196779	-2.483939	0.030118
H	-6.015845	-3.194145	0.027440
H	-5.860010	3.036920	0.703843
H	0.053010	4.519495	-0.637906
H	-0.207440	-0.639651	-0.051123
H	-2.350324	1.513834	0.049442
C	4.279013	1.683771	-0.318759
C	4.753702	0.421995	0.049232
C	5.400097	2.547107	-0.527977
C	6.227941	0.512092	0.094261
C	3.890548	-0.670429	0.316345
C	6.565996	1.840837	-0.302429
H	5.338205	3.590626	-0.807264
C	7.141800	-0.456305	0.468565
C	4.330783	-1.858790	0.933997
H	7.575192	2.219795	-0.380356
C	6.868091	-1.730556	0.976762
H	8.190397	-0.177833	0.399527
C	5.623662	-2.309168	1.212823
H	3.549356	-2.528104	1.266328

H	7.729226	-2.328171	1.258933
H	5.659847	-3.284015	1.692298

S-5,6-HP			
C	3.109061	-3.409489	0.256348
C	2.437480	-4.638077	0.503957
C	1.088492	-4.376100	0.586198
C	0.896838	-2.979586	0.398521
N	2.142461	-2.426607	0.225721
H	2.405635	-1.468144	0.013918
H	2.925582	-5.596047	0.597129
H	0.297743	-5.086918	0.764840
C	-0.335953	-2.302733	0.346709
C	-1.620285	-2.895024	0.323440
C	-2.556439	-1.881280	0.157986
C	-1.835039	-0.646017	0.104642
N	-0.502541	-0.937135	0.226088
H	-1.812197	-3.953451	0.394023
C	-1.689969	1.798344	0.371318
C	-2.258406	3.015706	0.930025
C	-1.214318	3.853689	1.150026
H	-1.236747	4.848498	1.571745
C	-2.435097	0.617951	0.051242
C	-0.019820	3.148909	0.725401
N	-0.334605	1.884218	0.296352
C	4.416412	2.472350	-0.357159
C	2.509816	3.498400	0.323522
C	3.535706	4.484553	0.202117
H	5.636464	4.324287	-0.436105
H	3.388346	5.532832	0.412944
C	5.448235	0.139831	-0.631726
C	6.714361	-0.550725	-0.859538
C	6.480507	-1.863788	-0.632474
C	5.070239	-1.969953	-0.291503
N	4.462463	-0.742590	-0.308124
H	7.643528	-0.071811	-1.133889
H	7.174480	-2.690415	-0.686278
C	1.206401	3.814760	0.706703
C	4.677477	3.871411	-0.236002
C	5.399244	1.536063	-0.672367
N	3.087167	2.291796	-0.027604
C	4.460919	-3.188884	0.006272
H	5.096047	-4.066953	0.016274
H	6.346058	2.001342	-0.925774

H	1.125863	4.853501	1.011756
H	0.177395	-0.181645	0.256788
H	2.620101	1.398736	-0.024315
H	-3.294596	3.179706	1.176925
C	-3.878875	0.635552	-0.255414
C	-4.452938	1.834875	-0.738951
C	-4.596286	-0.582207	-0.165095
C	-5.783227	2.157422	-0.997759
H	-3.751390	2.628659	-0.955764
C	-6.046056	-0.848218	-0.290178
C	-3.978598	-1.820750	0.069251
C	-6.950655	1.400356	-0.888126
H	-5.933988	3.176445	-1.344603
C	-7.066633	0.045662	-0.570662
C	-6.224031	-2.246308	-0.082319
C	-4.985727	-2.831256	0.112701
H	-7.875298	1.919380	-1.119607
H	-8.071869	-0.368493	-0.582110
H	-7.178620	-2.752783	-0.101490
H	-4.804162	-3.887126	0.263925

S-5,6-PH			
C	2.686052	-3.583449	-0.262901
C	1.859202	-4.711847	-0.472327
C	0.547500	-4.276018	-0.514757
C	0.546573	-2.871892	-0.335402
N	1.853718	-2.482981	-0.201884
H	2.244585	-1.562682	-0.020971
H	2.215326	-5.725516	-0.573374
H	-0.332077	-4.881261	-0.663886
C	-0.596153	-2.032553	-0.268913
C	-1.932444	-2.462574	-0.221890
C	-2.746699	-1.333500	-0.089795
C	-1.888096	-0.203263	-0.073501
N	-0.601594	-0.656236	-0.184574
H	-2.241036	-3.494358	-0.258959
C	-1.447483	2.221379	-0.265969
C	-1.849359	3.564396	-0.636412
C	-0.704648	4.278665	-0.769843
H	-0.596381	5.316035	-1.053117
C	-2.331698	1.137456	-0.042067
C	0.390256	3.369112	-0.477545
N	-0.078531	2.121085	-0.209590
C	4.774046	2.082855	0.318922
C	2.964335	3.372931	-0.163193
C	4.114452	4.223227	-0.042312
H	6.211473	3.774909	0.433439

H	4.080711	5.294482	-0.170502
C	5.517761	-0.368634	0.460653
C	6.698162	-1.215801	0.600755
C	6.281667	-2.488214	0.401630
C	4.850951	-2.411345	0.160194
N	4.410403	-1.107520	0.209392
H	7.697937	-0.861282	0.807475
H	6.865367	-3.397593	0.414760
C	1.701511	3.875011	-0.438632
C	5.194348	3.453665	0.268484
C	5.649765	1.029560	0.527016
N	3.413738	2.083339	0.066371
C	4.071167	-3.533606	-0.083336
H	4.584076	-4.488069	-0.118555
H	6.663070	1.364377	0.721999
H	1.736950	4.943540	-0.626048
H	0.162138	0.016835	-0.216231
H	2.845040	1.252176	0.034687
H	-2.853299	3.900476	-0.832556
C	-3.760810	1.261750	0.175152
C	-4.630359	0.145722	0.160763
C	-4.556652	2.405930	0.501152
C	-5.997592	0.641964	0.423144
C	-4.188603	-1.180124	0.012246
C	-5.885815	2.039624	0.631076
H	-4.177903	3.402001	0.669885
C	-7.180668	-0.082137	0.472604
C	-5.008494	-2.327653	-0.024625
H	-6.708864	2.697510	0.871827
C	-7.362169	-1.455387	0.305694
H	-8.079351	0.499169	0.664445
C	-6.389424	-2.435980	0.088004
H	-4.487191	-3.268637	-0.161379
H	-8.385228	-1.812041	0.367825
H	-6.772976	-3.449500	0.006834

S-7,7-HP			
C	0.397758	-2.945680	-0.185645
C	1.790513	-3.090511	-0.334845
C	2.386820	-1.831610	-0.258370
C	1.327413	-0.898014	-0.053206
N	0.144360	-1.600307	-0.033560
H	-0.800097	-1.271991	0.138065
H	2.287542	-4.037256	-0.473351
C	1.447613	0.493223	0.016566
C	2.640281	1.284799	0.130407
C	2.222563	2.616622	0.046858

C	0.824185	2.662968	-0.073430
N	0.383355	1.359197	-0.059654
C	-1.373480	3.841777	-0.289936
C	-2.095207	5.096568	-0.434251
C	-3.408267	4.774325	-0.437159
H	-4.261334	5.432683	-0.519610
C	0.010999	3.791684	-0.210327
C	-3.477912	3.322363	-0.288970
N	-2.239724	2.775729	-0.215777
C	-5.331180	-0.845232	0.293660
C	-5.169614	1.400968	-0.002841
C	-6.555437	1.060607	0.151845
H	-7.545336	-0.870385	0.491516
H	-7.355768	1.784268	0.123490
C	-3.937987	-3.005676	0.293005
C	-4.072655	-4.460356	0.311499
C	-2.829661	-4.960904	0.130937
C	-1.943569	-3.811406	0.025925
N	-2.644870	-2.633384	0.130331
H	-5.002402	-4.997742	0.432800
H	-2.520304	-5.994905	0.077568
C	-4.735818	2.702862	-0.194807
C	-6.651388	-0.284590	0.340847
C	-5.088374	-2.205822	0.393511
N	-4.465134	0.214539	0.094446
C	-0.572835	-3.950664	-0.144462
H	-0.196165	-4.962822	-0.238454
H	-6.000110	-2.775656	0.538867
H	-5.563213	3.402223	-0.254486
H	-0.603594	1.149308	-0.166443
H	-3.464354	0.128537	0.005017
H	-1.640297	6.073433	-0.514981
H	0.535880	4.739149	-0.253454
H	2.847879	3.493958	0.039751
C	4.050991	0.887183	0.320538
C	4.857166	1.917907	0.881030
C	4.535421	-0.383629	-0.046983
C	6.228560	2.070899	1.014224
H	4.294430	2.749728	1.282129
C	5.982012	-0.750093	-0.210147
C	3.798578	-1.553464	-0.392100
C	7.273709	1.237350	0.614444
H	6.530839	2.999550	1.491360
C	7.140077	-0.021672	0.048950
C	6.019369	-2.069603	-0.698195
C	4.724022	-2.552060	-0.784636
H	8.282131	1.600910	0.779872
H	8.064358	-0.540894	-0.193612
H	6.924078	-2.610005	-0.938755
H	4.451932	-3.549233	-1.101404

S-7,7-PH

C	-0.823905	2.662823	-0.073646
C	-2.222292	2.616551	0.046749
C	-2.640122	1.284786	0.130259
C	-1.447467	0.493097	0.016107
N	-0.383190	1.359050	-0.060265
H	0.603674	1.149044	-0.167481
H	-2.847525	3.493956	0.039966
C	-1.327389	-0.898111	-0.053605
C	-2.386982	-1.831643	-0.258528
C	-1.790872	-3.090627	-0.334873
C	-0.398082	-2.945984	-0.185562
N	-0.144459	-1.600601	-0.033816
C	1.943184	-3.811701	0.026143
C	2.829406	-4.961092	0.131070
C	4.072319	-4.460405	0.311776
H	5.002111	-4.997694	0.433153
C	0.572431	-3.951036	-0.144235
C	3.937523	-3.005737	0.293113
N	2.644341	-2.633598	0.130457
C	5.169785	1.400978	-0.002698
C	5.330857	-0.845263	0.293653
C	6.651198	-0.284948	0.340531
H	7.356038	1.783783	0.123378
H	7.545031	-0.870985	0.490932
C	3.478245	3.322395	-0.288990
C	3.408502	4.774372	-0.436887
C	2.095417	5.096503	-0.434150
C	1.373780	3.841633	-0.290019
N	2.240061	2.775651	-0.215862
H	4.261533	5.432802	-0.519143
H	1.640432	6.073336	-0.514816
C	5.087877	-2.205853	0.393457
C	6.555533	1.060315	0.151789
C	4.736134	2.702929	-0.194742
N	4.465024	0.214719	0.094700
C	-0.010717	3.791524	-0.210427
H	-0.535571	4.739012	-0.253372
H	5.563557	3.402245	-0.254556
H	5.999618	-2.775729	0.538634
H	0.800133	-1.272453	0.137468
H	3.464188	0.129141	0.005524
H	2.520186	-5.995132	0.077693

H	0.195772	-4.963198	-0.238217
H	-2.288039	-4.037325	-0.473163
C	-3.798706	-1.553288	-0.392207
C	-4.535384	-0.383418	-0.046963
C	-4.724314	-2.551751	-0.784782
C	-5.982012	-0.749624	-0.210155
C	-4.050759	0.887265	0.320706
C	-6.019575	-2.069128	-0.698239
H	-4.452314	-3.548926	-1.101602
C	-7.139953	-0.020959	0.048818
C	-4.856699	1.917882	0.881733
H	-6.924389	-2.609361	-0.938794
C	-7.273364	1.238003	0.614505
H	-8.064321	-0.539904	-0.193991
C	-6.228069	2.071161	1.014763
H	-4.293777	2.749431	1.283138
H	-8.281725	1.601804	0.779774
H	-6.530204	2.999715	1.492179

Hx-1,2-HP			
C	8.407539	-0.852567	0.183329
H	9.411862	-0.460205	0.234834
C	8.023452	-2.162569	0.126788
H	8.094877	1.876962	0.245082
C	7.150792	1.347434	0.191816
C	5.907875	3.570292	0.178979
C	7.220381	-0.041087	0.160111
C	4.595653	3.892623	0.118790
C	5.971791	2.107320	0.154906
H	6.754088	4.240675	0.237078
C	6.587091	-2.203275	0.069140
C	5.789253	-3.337426	-0.000362
C	3.860163	2.623031	0.059289
H	6.315364	-4.285312	-0.018183
H	4.176121	4.884584	0.125541
C	1.388848	4.724402	-0.137946
N	4.737857	1.574381	0.087280
C	2.494432	2.368782	-0.004258
C	1.404017	3.257975	-0.067718
C	0.087095	5.089269	-0.184328
N	6.152615	-0.900623	0.093027
C	4.386736	-3.381269	-0.051296
C	-0.684851	3.849629	-0.142093
H	2.242932	5.380127	-0.160186
N	3.584365	-2.297280	-0.025470
N	0.143815	2.769496	-0.076979
C	3.602305	-4.611339	-0.134426

C	2.302886	-2.765836	-0.101530
C	1.225840	-1.875616	-0.067909
C	-2.068452	3.776171	-0.157089
C	2.303906	-4.229748	-0.168071
H	-0.322009	6.088110	-0.244257
C	-0.145660	-2.136618	-0.204068
H	2.225688	1.318657	-0.003065
N	-1.058599	-1.147149	0.009707
N	-2.419179	1.316474	-0.051867
C	-2.865669	2.619202	-0.111400
C	-0.826865	-3.372462	-0.572912
H	1.486121	-0.836937	0.103039
C	-2.281342	-1.704506	-0.147185
H	4.000177	-5.616449	-0.151040
H	-1.441597	1.023406	-0.021299
C	-2.155749	-3.104327	-0.537446
C	-3.480788	-0.957339	0.008192
C	-3.479072	0.461575	0.000134
H	-2.615155	4.711652	-0.204072
H	5.176003	-0.603691	0.062833
H	1.442820	-4.875885	-0.196116
C	-4.278472	2.582565	-0.109351
H	-0.369099	-4.297726	-0.879998
C	-4.673827	1.249989	-0.034660
H	-2.953443	-3.769798	-0.824080
H	-4.902353	3.461482	-0.158201
H	8.656792	-3.036801	0.124215
C	-5.989141	0.631577	-0.002624
C	-7.135787	1.449818	-0.057704
C	-5.982451	-0.769894	0.100566
C	-8.480180	1.098864	-0.013256
H	-6.945812	2.513428	-0.148838
C	-7.119051	-1.693660	0.272438
C	-4.796566	-1.539862	0.139975
C	-9.086495	-0.152386	0.130906
H	-9.170158	1.934522	-0.091606
C	-8.475199	-1.398303	0.274060
C	-6.565173	-2.988910	0.450414
C	-5.187056	-2.896695	0.387231
H	-10.171625	-0.150161	0.147057
H	-9.142233	-2.247185	0.401916
H	-7.138485	-3.888013	0.626091
H	-4.510247	-3.721470	0.546768

Hx-1,2-PH			
C	8.253128	-1.201893	0.259037
H	9.276139	-0.872573	0.358963

C	7.797265	-2.488215	0.094921
H	8.091773	1.529193	0.497973
C	7.119617	1.062537	0.385628
C	6.017036	3.347448	0.442577
C	7.118244	-0.334409	0.269089
C	4.727145	3.745272	0.339438
C	6.002193	1.889327	0.351880
H	6.894509	3.965503	0.571312
C	6.372404	-2.440269	0.007135
C	5.503822	-3.524540	-0.169084
C	3.928752	2.522212	0.189786
H	5.980522	-4.493862	-0.266717
H	4.359150	4.756766	0.382535
C	1.605160	4.759768	-0.174059
N	4.728928	1.432249	0.210194
C	2.537940	2.352299	0.059002
C	1.524904	3.298240	-0.061709
C	0.332706	5.201610	-0.288663
N	6.007270	-1.123330	0.119610
C	4.115488	-3.489002	-0.233382
C	-0.519960	4.010953	-0.240948
H	2.500458	5.358516	-0.187483
N	3.367226	-2.356704	-0.096903
N	0.219671	2.893470	-0.113266
C	3.257564	-4.649516	-0.443378
C	2.078220	-2.737120	-0.221454
C	1.042181	-1.783655	-0.077208
C	-1.920795	4.037937	-0.304126
C	1.985444	-4.183497	-0.441141
H	-0.009921	6.220964	-0.399513
C	-0.320201	-1.937512	-0.268581
H	2.208640	1.319600	0.048263
N	-1.191759	-0.921902	0.079107
N	-2.407201	1.625291	-0.104871
C	-2.784159	2.949965	-0.235453
C	-1.071220	-3.061532	-0.816518
H	1.363722	-0.801120	0.249996
C	-2.423708	-1.374140	-0.158723
H	3.591433	-5.670781	-0.561890
H	-1.445446	1.295714	-0.025657
C	-2.379357	-2.715728	-0.753437
C	-3.599266	-0.562404	0.042325
C	-3.514456	0.833524	-0.028814
H	-2.393987	5.008296	-0.403147
H	5.048715	-0.771500	0.090437
H	1.083664	-4.765227	-0.535027
C	-4.209372	2.990894	-0.267054
H	-0.664625	-3.958906	-1.252367
C	-4.675005	1.698339	-0.132238
H	-3.219203	-3.275052	-1.135418

H	-4.789280	3.893969	-0.379254
H	8.383203	-3.393032	0.039215
C	-4.937546	-1.138207	0.251226
C	-5.031247	-2.478565	0.687886
C	-6.066477	-0.291325	0.107771
C	-6.147141	-3.293059	0.875985
H	-4.091029	-2.953344	0.933225
C	-7.507811	-0.605695	0.151568
C	-5.961277	1.089114	-0.107634
C	-7.507979	-3.037430	0.711066
H	-5.910962	-4.300848	1.207144
C	-8.120677	-1.825093	0.384798
C	-8.202530	0.620909	-0.078674
C	-7.279037	1.636980	-0.215855
H	-8.172642	-3.875529	0.894899
H	-9.206964	-1.828726	0.343055
H	-9.278232	0.718609	-0.114168
H	-7.508538	2.682716	-0.371376

Hx-2,3-HP			
C	7.822139	-2.037320	0.399617
H	8.876196	-1.872809	0.564345
C	7.191236	-3.225096	0.133224
H	8.057251	0.668717	0.791078
C	7.032312	0.359022	0.620342
C	6.277091	2.786506	0.725787
C	6.828543	-1.005881	0.419056
C	5.066218	3.377837	0.578950
C	6.047575	1.350725	0.590723
H	7.230396	3.262178	0.908996
C	5.791410	-2.956667	-0.013824
C	4.783432	-3.884173	-0.295905
C	4.103329	2.294461	0.368009
H	5.108908	-4.910633	-0.422059
H	4.848551	4.431495	0.640230
C	2.188330	4.836669	-0.255028
N	4.733127	1.091660	0.394763
C	2.715529	2.334827	0.172647
C	1.869438	3.422257	-0.049611
C	1.011429	5.456169	-0.511303
N	5.620352	-1.610830	0.169932
C	3.420100	-3.623618	-0.419658
C	-0.015711	4.418150	-0.451141
H	3.167659	5.285816	-0.241254
N	2.852657	-2.399830	-0.270716
N	0.526209	3.215637	-0.174923
C	2.402589	-4.635149	-0.706777

C	1.515756	-2.576287	-0.422285
C	0.642316	-1.483863	-0.293933
C	-1.384842	4.635854	-0.661976
C	1.216600	-3.986378	-0.709212
H	0.844341	6.501912	-0.728790
C	-0.753468	-1.457547	-0.274683
H	2.229394	1.365986	0.169603
N	-1.396351	-0.239840	-0.134755
N	-2.317102	2.376157	-0.242647
C	-2.415216	3.708490	-0.581436
C	-1.714826	-2.541326	-0.319858
H	1.123266	-0.522109	-0.160795
C	-2.699726	-0.518274	-0.066897
H	2.587166	-5.685214	-0.885411
H	-1.443365	1.864694	-0.093515
C	-2.947488	-1.965697	-0.178851
C	-3.772757	0.409722	0.039846
C	-3.555971	1.790258	-0.217605
H	-1.689843	5.646966	-0.909173
H	4.725908	-1.119349	0.123790
H	0.248164	-4.413073	-0.907788
C	-3.801725	3.969452	-0.816965
H	-1.502178	-3.592357	-0.409106
C	-4.495886	2.809864	-0.603809
H	-4.198627	4.922105	-1.133645
H	7.637751	-4.203634	0.042907
H	-5.549585	2.656287	-0.758957
C	-5.112288	-0.131274	0.339678
C	-6.086289	0.726285	0.892519
C	-5.323229	-1.525503	0.166812
C	-7.437307	0.509078	1.169773
H	-5.734511	1.709882	1.170863
C	-6.568526	-2.315339	0.254358
C	-4.291342	-2.429202	-0.124033
C	-8.237987	-0.617214	0.997313
H	-7.949447	1.372134	1.587005
C	-7.845099	-1.892449	0.581268
C	-6.217251	-3.667786	-0.038952
C	-4.854010	-3.739140	-0.242314
H	-9.285292	-0.499030	1.256664
H	-8.621632	-2.652603	0.552934
H	-6.917563	-4.490595	-0.064266
H	-4.291758	-4.640116	-0.448442

Hx-2,3-PH			
C	-7.617269	-2.481565	0.265710
H	-8.684683	-2.396572	0.402222

C	-6.892092	-3.615940	0.029288
H	-8.065810	0.206556	0.640021
C	-7.018137	-0.028091	0.492241
C	-6.441982	2.448149	0.631223
C	-6.704349	-1.371623	0.300824
C	-5.278851	3.129940	0.520817
C	-6.101485	1.031221	0.484328
H	-7.432666	2.847581	0.798004
C	-5.508167	-3.243793	-0.084579
C	-4.434034	-4.089841	-0.322579
C	-4.228411	2.124152	0.315573
H	-4.675714	-5.140277	-0.440428
H	-5.145755	4.196243	0.598220
C	-2.504790	4.837009	-0.121259
N	-4.773510	0.873176	0.312246
C	-2.852843	2.273891	0.151663
C	-2.078902	3.437062	0.005261
C	-1.376714	5.561080	-0.301058
N	-5.449397	-1.881693	0.089041
C	-3.078968	-3.727918	-0.413531
C	-0.270715	4.604367	-0.277942
H	-3.515819	5.208569	-0.105201
N	-2.614918	-2.469881	-0.276560
N	-0.731696	3.339844	-0.094172
C	-1.984807	-4.665327	-0.651490
C	-1.253947	-2.545850	-0.390275
C	-0.482214	-1.388122	-0.272204
C	1.069107	4.939329	-0.430625
C	-0.846995	-3.929816	-0.636508
H	-1.287064	6.628881	-0.444090
C	0.913821	-1.235078	-0.226392
H	-2.294157	1.346058	0.111996
N	1.463510	0.022125	-0.161277
N	2.173404	2.729316	-0.181509
C	2.177808	4.082655	-0.396550
C	1.948536	-2.239640	-0.178450
H	-1.045749	-0.466133	-0.184518
C	2.788752	-0.150276	-0.068536
H	-2.085798	-5.729166	-0.815766
H	1.337995	2.148579	-0.078747
C	3.142008	-1.565899	-0.072345
C	3.784131	0.865305	-0.001034
C	3.459124	2.236950	-0.181349
H	1.301792	5.986616	-0.589714
H	-4.597428	-1.319116	0.060645
H	0.153431	-4.290663	-0.808207
C	3.538307	4.470434	-0.569803
H	1.800257	-3.305858	-0.185659
C	4.318838	3.347441	-0.442533
H	3.866598	5.476502	-0.782184

H	-7.259392	-4.627042	-0.061381
H	5.384395	3.296268	-0.576603
C	4.515431	-2.017752	0.039754
C	4.796748	-3.398404	-0.003042
C	5.464550	-0.989577	0.204763
C	6.010023	-4.065391	0.116456
H	3.936346	-4.040971	-0.153367
C	6.906502	-1.100585	0.473008
C	5.129467	0.387647	0.224931
C	7.297030	-3.569819	0.346741
H	5.945035	-5.146431	0.028915
C	7.692835	-2.245216	0.521923
C	7.384100	0.219603	0.689890
C	6.327832	1.100683	0.556444
H	8.083773	-4.314709	0.411060
H	8.749153	-2.082422	0.720557
H	8.404205	0.476192	0.937770
H	6.399613	2.162747	0.729559

Hx-4,4-HP			
N	3.873006	-1.860847	-0.335072
N	3.174310	2.815528	0.142018
N	-0.928853	2.143195	0.027546
N	-0.190145	-2.463698	0.180344
N	0.870311	4.521341	0.274912
N	2.215798	-4.183900	-0.068741
C	3.424152	-4.795162	-0.293569
C	4.636001	-4.154475	-0.541051
C	4.847015	-2.771824	-0.551589
C	4.475497	-0.640304	-0.352745
C	3.710400	0.508944	-0.137090
C	4.112780	1.842021	0.006395
C	3.848614	3.980210	0.287872
C	3.230538	5.224229	0.428255
C	1.856728	5.465980	0.413049
C	-0.363899	5.122992	0.254361
C	-1.852387	3.126524	-0.041349
C	-1.595936	4.495804	0.093708
C	-1.601122	0.964143	-0.081592
C	-0.842448	-0.206154	0.013826
C	-1.189433	-1.537489	0.223398
C	1.248331	-5.122273	0.192005
C	-0.091912	-4.883496	0.473392
C	-0.760022	-3.650584	0.484592
C	6.139042	-2.115256	-0.749074
C	5.910665	-0.787473	-0.621328
C	5.459474	2.420230	0.081010
C	5.292245	3.751204	0.260447
C	1.206928	6.740270	0.501833

C	-0.142452	6.532386	0.401058
C	-3.041614	1.208753	-0.332396
C	-3.164725	2.571303	-0.279473
C	-2.164522	-3.490104	0.777943
C	-2.476564	-2.164736	0.618880
C	3.204296	-6.209224	-0.183732
C	1.886018	-6.407505	0.121024
H	7.076579	-2.611353	-0.957763
H	6.633023	0.005025	-0.724703
H	2.642178	0.340791	-0.054158
H	6.394524	1.887476	0.033556
H	6.055992	4.508295	0.370369
H	1.047243	3.520256	0.187404
H	0.227338	-0.033714	-0.030886
H	-2.842930	-4.291258	1.030911
H	-0.685700	-5.763853	0.693242
H	2.073187	-3.173591	-0.080469
H	1.379045	-7.346875	0.281561
H	3.972181	-6.956628	-0.313803
H	5.492129	-4.798266	-0.707014
H	1.723547	7.680775	0.618709
H	3.866395	6.094950	0.540657
H	-0.928071	7.272353	0.422455
H	-4.076597	3.139948	-0.390799
H	-2.454131	5.158122	0.065854
C	-4.238575	0.392653	-0.653156
C	-5.035069	0.976637	-1.665231
C	-4.615047	-0.750569	0.094702
C	-6.374052	0.810051	-2.018075
H	-4.508882	1.707041	-2.267799
C	-6.045763	-1.079426	0.403979
C	-3.829528	-1.668155	0.832692
C	-7.375955	0.109854	-1.360195
H	-6.685921	1.372101	-2.894250
C	-7.216642	-0.679776	-0.221247
C	-6.029843	-2.042155	1.442129
C	-4.722300	-2.416185	1.663443
H	-8.381403	0.198073	-1.758281
H	-8.124806	-1.107131	0.197177
H	-6.911109	-2.452101	1.914846
H	-4.398291	-3.182969	2.353492

5. Magnitudes of different transition dipole moment vector:-

System	f	μ^{00}	μ^{ff}	μ^{ii}	μ^{if}	μ^{fi}	μ^{oi}	μ^{io}	μ^{of}	μ^{fo}
Pr-1,2-HP	5	0.63	0.59	0.52	3.24	1.21	2.19	1.54	2.44	2.19
Pr-1,2-PH	5	0.43	1.04	0.20	1.91	1.23	1.77	1.34	2.95	2.76
NCP-1,2-HP	5	0.73	1.41	1.36	3.15	1.65	2.47	1.75	2.66	3.04
NCP-1,2-PH	5	0.60	0.82	0.47	0.36	0.36	2.19	1.73	3.04	1.93
SP-1,2-HP	4	1.27	1.17	1.25	1.25	0.50	1.35	0.97	1.88	1.19
	5	1.27	1.37	1.25	2.10	0.11	1.35	0.97	2.49	1.55
SP-1,2-PH	4	1.24	1.17	1.12	1.86	1.34	1.18	0.85	0.66	0.43
	5	1.24	1.27	1.12	0.32	0.46	1.18	0.85	3.45	2.21
S-5,6-HP	5	0.31	0.92	0.36	2.06	0.90	3.03	2.49	2.98	2.63
S-5,6-PH	5	0.94	1.62	1.04	3.32	1.93	3.08	2.09	2.65	3.45
Hx-2,3-HP	4	0.77	3.74	1.27	0.59	0.29	2.15	1.55	3.08	2.21
	5	0.77	1.06	1.27	2.67	1.47	2.15	1.55	2.89	2.35
Hx-2,3-PH	4	1.04	1.15	0.64	2.54	1.86	2.75	2.01	4.56	2.55
	5	1.04	0.58	0.64	0.14	11.98	2.75	2.01	5.38	2.77

Table S2: Different transition dipole moment vectors involved for porphyrinoid-azulene systems.

6. Two-photon absorption cross section:-

System	1st	2nd	3rd	4th	5th
Pr	0	0	0	0	0
Pr-1,2-HP	1433	3981	2815	74352	399499
Pr-1,2-PH	538	5052	18427	61804	47444
NCP	19	14	12	52	1297
NCP-1,2-HP	2808	2683	1421	99513	539020
NCP-1,2-PH	1401	5668	27593	80415	5192
SP	610	614	25	17	1
SP-1,2-HP	89	4663	4401	33075	16347
SP-1,2-PH	106	6669	712	35877	1252

S	2,100	862	67	112	NA
S-1,2-HP	1,535	10,124	17,882	1,33,074	95,238
S-2,3-PH	1,453	11,362	8,936	8,080	2,18,966
S-4,5-HP	8,265	34,091	319	23,285	1,33,563
S-4,5-PH	3,282	42,735	5,778	1,29,499	4,710
S-5,6-HP	1297	24184	14124	178277	60752
S-5,6-PH	17368	10559	3501	179961	1687515
S-7,7-HP	962	5,201	5,879	90,533	82,284
S-7,7-PH	955	5,184	5,876	90,518	82,301
Hx	0	0	0	0	0
Hx-1,2-HP	64,002	10,479	70,746	5,38,030	50558
Hx-1,2-PH	64002	10479	70746	538030	50558
Hx-2,3-HP	20,038	14,084	4,380	21,88,878	3,34,337
Hx-2,3-PH	2496	28346	11972	58818	473426
Hx-4,4-HP	1,792	12,209	2,413	31,862	7,956

Table S3: TPA transition strength of the first five singlet excited states of all the systems computed at RICC2/cc-pVDZ level of theory.