Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Materials

Contrasting the excited state properties of different conformers of *trans*- and *cis*- 2, 2′-Bipyridine oligomers in the gas phase

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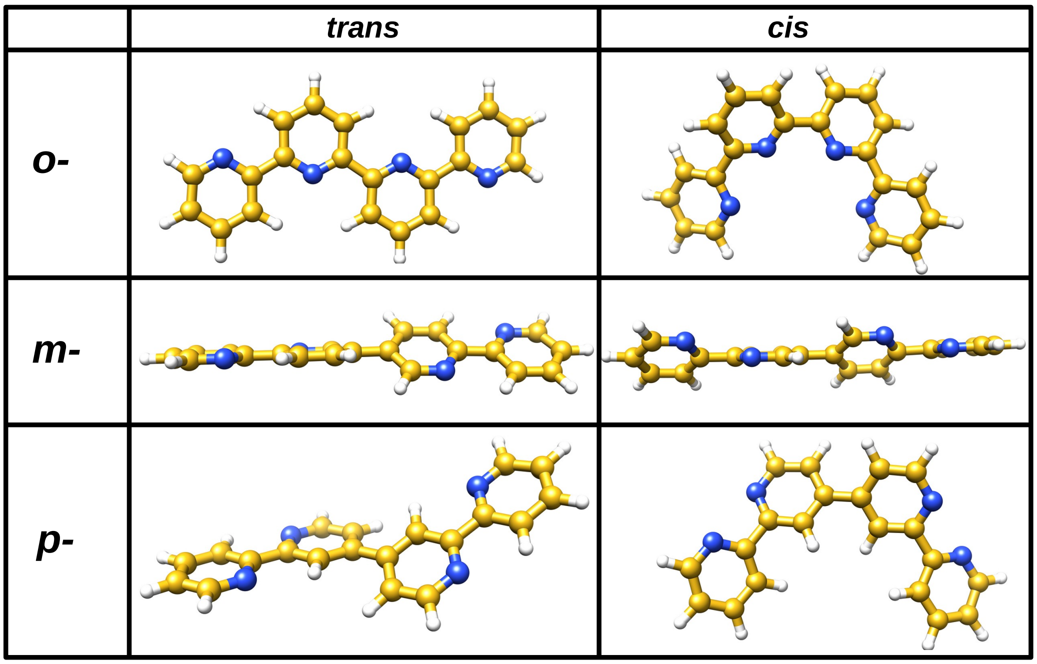

Figure S1: Ground state optimized structures of ***trans***- and ***cis***-$(\mathbf{BPY})_2$ for ***o-***, ***m-***, and ***p-*** conformers obtained at B3LYP-D3/def2-SVPD level.

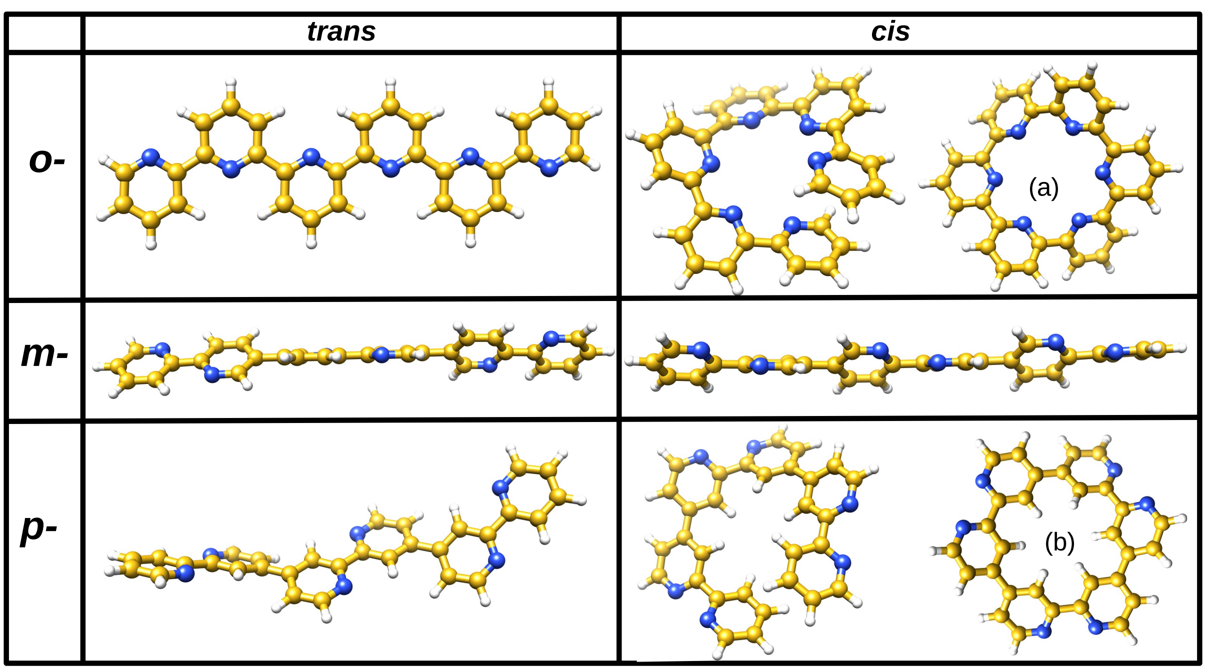

Figure S2: Optimized geometries of ***trans***- and ***cis***-$(\mathbf{BPY})_3$ for ***o-***, ***m-***, and ***p-*** conformers. In this figure, (a) and (b) are the cyclic (cy) analogs of ***o-*** and ***p-*** conformers, respectively.

Table S1: Energies (in eV) of ground state optimized structures of all the oligomers at B3LYP-D3/def2-SVPD level

trans	**(BPY)**$_2$	**(BPY)**$_3$	**(BPY)**$_4$
o-	0.00	0.00	0.00
m-	0.19	0.38	0.57
p-	0.17	0.33	0.50
cis			
o-	0.91	1.38	0.50
cy-***o-***		33.91	
m-	0.88	1.28	1.77
p-	0.86	1.12	1.04
cy-***p-***		33.67	

In the case of ***trans*** oligomers for ***o-*** conformer, only one type of the dihedral angle ϕ_i, defined as ∠N-C-C-C, is used. In ***m-*** and ***p-***, two types of dihedral angles, ϕ_j and ϕ_k, are used which are defined as ∠N-C-C-C and ∠C-C-C-C, respectively. Similarly, in the case of ***cis-o-*** conformer, only one type of dihedral angle ϕ_i=∠N-C-C-N is used, whereas for ***m-*** and ***p-*** two types of dihedral angles ϕ_j=∠N-C-C-N and ϕ_k=∠C-C-C-C are used. In the case of tetramers, for example, i=1-7, j=1, 3, 5, 7, and k=2, 4, 6.

Table S2: Calculated dihedral angles (ϕ_{1-7}) of (BPY)$_2$-(BPY)$_4$ for *trans*- structures of *o-* conformer at B3LYP-D3/def2-SVPD level

Angle	**(BPY)**$_2$	**(BPY)**$_3$	**(BPY)**$_4$
ϕ_1	0	0	0
ϕ_2	0	0	0
ϕ_3	0	0	0
ϕ_4		0	0
ϕ_5		0	0
ϕ_6			0
ϕ_7			0

Table S3: Calculated dihedral angles (ϕ_{1-7}) of $(\mathbf{BPY})_2$-$(\mathbf{BPY})_4$ for *trans*- structures of *m*- and *p*- conformers at B3LYP-D3/def2-SVPD level

	m-			***p-***		
Angle	$(\mathbf{BPY})_2$	$(\mathbf{BPY})_3$	$(\mathbf{BPY})_4$	$(\mathbf{BPY})_2$	$(\mathbf{BPY})_3$	$(\mathbf{BPY})_4$
ϕ_1	0	0	0	-0.8	-0.8	0.6
ϕ_2	37.2	-37	37.1	33.7	33.6	-33.3
ϕ_3	0	0	0	-0.5	-1.6	1.6
ϕ_4		37	37.2		33.6	-33.5
ϕ_5		0	0		0.5	1.6
ϕ_6			37.1			-33.3
ϕ_7			0			0.8

Table S4: Calculated dihedral angles (ϕ_{1-7}) of $(\mathbf{BPY})_2$-$(\mathbf{BPY})_4$ for *cis*- structures of *o*- conformer at B3LYP-D3/def2-SVPD level

	o-			
Angle	$(\mathbf{BPY})_2$	$(\mathbf{BPY})_3$	cy-$(\mathbf{BPY})_3$	$(\mathbf{BPY})_4$
ϕ_1	39.6	-30.3	-26.5	38.7
ϕ_2	-38.4	20.8	-26.5	-26.0
ϕ_3	39.6	-44.6	51.7	53.3
ϕ_4		20.8	-26.5	-38.6
ϕ_5		-30.3	-26.5	53.3
ϕ_6			51.7	-26.0
ϕ_7				38.7

Table S5: Calculated dihedral angles (ϕ_{1-7}) of $(\mathbf{BPY})_2$-$(\mathbf{BPY})_4$ for *cis*- structures of *m*- and *p*- conformers at B3LYP-D3/def2-SVPD level

	m-			***p-***			
Angle	$(\mathbf{BPY})_2$	$(\mathbf{BPY})_3$	$(\mathbf{BPY})_4$	$(\mathbf{BPY})_2$	$(\mathbf{BPY})_3$	cy-$(\mathbf{BPY})_3$	$(\mathbf{BPY})_4$
ϕ_1	35.2	35.3	35.2	-37.3	-40.0	-17.5	-42.5
ϕ_2	-37.9	-37.7	-37.8	35.7	26.8	-23.9	29.0
ϕ_3	35.2	33.2	33.0	-37.3	-42.2	41.6	-42
ϕ_4		-37.8	-37.8		26.8	-23.9	22.3
ϕ_5		35.3	33.1		-40.0	-17.5	-42.0
ϕ_6			-37.8			39.0	29.0
ϕ_7			35.2				-42.5

Table S6: Vertical excitation energies (E_g), oscillator strengths (f_{osc}) and the rotatory strengths (R in 10^{-40} erg-esu-cm/Gauss) of first sixteen excited states for three conformers of *trans*- and *cis*-$(BPY)_2$ obtained at RI-ADC(2)/def2-TZVPD level

trans		***o-***				***m-***				***p-***		
State	irrep	E_g	f_{osc}	R	irrep	E_g	f_{osc}	R	irrep	E_g	f_{osc}	R
S_1	A	4.37	0.000	0.00	B	4.19	1.487	-1.68	A	4.33	0.005	-6.41
S_2	B	4.37	0.000	0.00	A	4.20	0.002	-1.80	B	4.34	0.013	29.95
S_3	A	4.39	0.000	0.00	B	4.38	0.292	28.89	A	4.51	0.014	-11.13
S_4	B	4.46	0.460	0.00	A	4.62	0.000	1.84	B	4.55	0.298	102.66
S_5	A	4.48	0.004	0.00	A	4.64	0.001	2.40	A	4.64	0.000	2.56
S_6	B	4.70	0.000	0.00	B	4.73	0.036	-56.86	B	4.66	0.060	-160.54
S_7	B	4.78	0.696	0.00	B	4.75	0.010	-62.68	B	4.80	0.637	-235.95
S_8	B	4.79	0.000	0.00	A	4.82	0.001	-8.71	A	4.84	0.034	237.77
S_9	A	4.80	0.000	0.00	B	4.92	0.001	13.02	B	4.91	0.001	0.86
S_{10}	A	4.82	0.000	0.00	A	4.94	0.000	-2.53	A	4.91	0.000	-0.11
S_{11}	A	5.05	0.004	0.00	B	5.10	0.006	12.17	A	5.08	0.005	3.28
S_{12}	B	5.06	0.000	0.00	A	5.12	0.006	-10.70	B	5.08	0.000	-1.66
S_{13}	B	5.13	0.228	0.00	B	5.14	0.041	-21.79	B	5.30	0.113	-13.22
S_{14}	A	5.35	0.000	0.00	A	5.39	0.000	2.66	A	5.41	0.027	90.78
S_{15}	B	5.47	0.580	0.00	A	5.46	0.008	60.34	B	5.47	1.217	-127.51
S_{16}	A	5.74	0.000	0.00	B	5.91	0.070	-29.31	A	5.75	0.000	-1.82
cis												
S_1	A	4.38	0.000	0.55	B	4.28	0.301	-99.18	B	4.35	0.003	-7.50
S_2	B	4.44	0.001	-2.91	A	4.31	0.000	-4.22	A	4.36	0.005	37.99
S_3	A	4.47	0.000	0.67	B	4.48	0.781	-213.58	A	4.56	0.008	45.18
S_4	B	4.52	0.003	25.56	A	4.55	0.000	0.42	B	4.57	0.007	13.80
S_5	A	4.58	0.001	-14.94	B	4.59	0.383	310.76	B	4.68	0.065	22.93
S_6	B	4.59	0.010	-46.51	A	4.78	0.000	-2.55	A	4.75	0.134	-100.47
S_7	B	4.72	0.279	-68.46	B	4.79	0.076	108.99	B	4.77	0.001	-4.37
S_8	A	4.86	0.002	17.60	A	4.86	0.000	-4.24	A	4.77	0.012	-4.69
S_9	B	4.86	0.003	-6.70	A	4.90	0.000	0.01	B	4.91	0.003	0.00
S_{10}	A	4.89	0.121	89.00	B	4.90	0.005	17.34	A	4.91	0.001	8.11
S_{11}	B	5.07	0.015	-92.64	B	4.94	0.217	-84.32	B	5.06	0.202	132.95
S_{12}	A	5.10	0.118	23.02	A	5.06	0.015	-14.32	A	5.08	0.062	-46.53
S_{13}	B	5.31	0.095	9.21	B	5.10	0.022	23.01	B	5.42	0.101	35.92
S_{14}	A	5.58	0.476	215.72	A	5.52	0.002	11.30	B	5.52	0.944	-24.65
S_{15}	B	5.68	0.078	-19.81	A	5.68	0.003	5.81	A	5.59	0.457	-124.32
S_{16}	A	5.70	0.028	5.03	B	5.96	0.008	9.70	A	5.66	0.064	-29.72

Table S7: Vertical excitation energies (E_g), oscillator strengths (f_{osc}) and the rotatory strengths (R in 10^{-40} erg-esu-cm/Gauss) of first sixteen excited states for three conformers of *trans*- and *cis*-(BPY)$_3$ obtained at RI-ADC(2)/def2-TZVPD level

trans		***o-***				***m-***				***p-***		
State		E_g	f_{osc}	R	irrep	E_g	f_{osc}	R	irrep	E_g	f_{osc}	R
S_1	A	4.34	0.000	0.00	B	3.94	2.785	23.69	A	4.30	0.007	0.03
S_2	B	4.35	0.000	0.00	A	4.12	0.001	2.61	A	4.33	0.001	-10.91
S_3	A	4.36	0.000	0.00	B	4.25	0.065	-12.97	B	4.33	0.019	34.58
S_4	B	4.37	0.001	0.00	A	4.30	0.001	3.20	B	4.47	0.137	87.82
S_5	A	4.37	0.000	0.00	A	4.49	0.002	-9.67	A	4.48	0.015	-43.96
S_6	B	4.42	0.000	0.00	B	4.55	0.009	-1.30	B	4.53	0.317	71.28
S_7	A	4.43	0.000	0.00	A	4.56	0.000	4.76	A	4.55	0.044	133.02
S_8	B	4.46	1.230	-0.01	B	4.63	0.039	-11.91	B	4.56	0.381	-217.32
S_9	A	4.50	0.007	0.00	A	4.69	0.001	-1.23	A	4.64	0.001	-4.82
S_{10}	B	4.65	0.000	0.00	A	4.71	0.000	4.50	B	4.64	0.120	-244.57
S_{11}	A	4.75	0.000	0.00	B	4.73	0.056	199.77	B	4.81	0.534	-494.18
S_{12}	B	4.75	0.000	0.00	B	4.78	0.100	-22.73	A	4.83	0.123	565.32
S_{13}	B	4.78	0.744	-0.02	B	4.89	0.007	-35.00	A	4.90	0.000	-0.65
S_{14}	A	4.79	0.000	0.00	A	4.92	0.000	3.59	A	4.91	0.000	0.51
S_{15}	B	4.83	0.000	0.00	B	4.93	0.001	3.66	B	4.91	0.000	0.97
S_{16}	A	4.84	0.000	0.00	A	5.05	0.002	4.08	B	5.07	0.001	-1.19
cis												
S_1	B	3.98	0.000	-1.77	B	4.17	1.960	-274.92	B	4.31	0.007	24.89
S_2	A	3.98	0.000	-0.76	A	4.18	0.001	-5.16	A	4.31	0.000	5.00
S_3	B	4.15	0.000	-0.41	A	4.30	0.000	1.27	A	4.34	0.001	8.13
S_4	A	4.16	0.000	2.10	B	4.33	0.235	-5.04	B	4.37	0.008	35.70
S_5	A	4.31	0.000	-0.10	B	4.43	0.365	184.29	B	4.55	0.001	-21.27
S_6	B	4.34	0.002	-2.24	A	4.54	0.002	5.25	A	4.56	0.012	65.44
S_7	B	4.38	0.000	4.91	B	4.55	0.044	121.95	B	4.58	0.019	82.03
S_8	A	4.38	0.000	-1.56	A	4.67	0.011	-4.77	A	4.63	0.025	-42.42
S_9	A	4.44	0.001	15.75	B	4.76	0.115	27.44	B	4.71	0.211	-139.30
S_{10}	B	4.44	0.002	31.47	A	4.77	0.000	-1.28	A	4.73	0.034	5.35
S_{11}	B	4.51	0.049	-514.84	B	4.78	0.074	136.53	B	4.76	0.000	0.03
S_{12}	A	4.60	0.328	345.84	A	4.81	0.006	-22.97	A	4.76	0.000	-1.80
S_{13}	B	4.67	0.004	-0.06	B	4.84	0.015	-24.76	A	4.77	0.049	8.71
S_{14}	A	4.68	0.004	15.53	B	4.89	0.066	-61.39	B	4.79	0.004	4.83
S_{15}	B	4.85	0.176	-93.22	A	4.90	0.000	0.04	B	4.89	0.002	-3.79
S_{16}	A	4.88	0.001	2.05	A	4.91	0.000	0.01	A	4.89	0.000	9.38

Table S8: Vertical excitation energies (E_g), oscillator strengths (f_{osc}) and the rotatory strengths (R in 10^{-40} erg-esu-cm/Gauss) of first sixteen excited states for cy-*o*- and cy-*p*- conformers of *cis*-$(BPY)_3$ obtained at RI-ADC(2)/def2-TZVPD level

	cy- ***o-***				cy- ***p-***			
State	irrep	E_g	f_{osc}	R	irrep	E_g	f_{osc}	R
S_1	A	4.05	0.000	0.00	B	4.08	0.000	0.10
S_2	B	4.05	0.001	4.06	A	4.08	0.001	-0.37
S_3	B	4.18	0.000	1.96	A	4.30	0.020	3.20
S_4	A	4.18	0.000	0.56	B	4.33	0.026	-113.55
S_5	A	4.39	0.001	23.68	B	4.33	0.010	-46.02
S_6	B	4.40	0.000	7.25	A	4.34	0.012	90.82
S_7	B	4.40	0.000	7.42	B	4.39	0.017	121.59
S_8	A	4.40	0.000	0.00	A	4.44	0.161	-63.88
S_9	B	4.49	0.001	-16.16	B	4.49	0.003	-1.49
S_{10}	A	4.51	0.000	4.62	A	4.49	0.000	-4.52
S_{11}	A	4.52	0.012	200.15	B	4.60	0.154	24.71
S_{12}	A	4.54	0.000	0.00	A	4.67	0.061	-44.97
S_{13}	B	4.55	0.014	31.24	B	4.69	0.013	12.29
S_{14}	B	4.62	0.348	-452.78	A	4.69	0.004	6.79
S_{15}	A	4.82	0.000	0.00	A	4.72	0.006	-1.60
S_{16}	B	4.83	0.354	317.22	B	4.76	0.023	3.83

Table S9: E_g, f_{osc}, Rotatory Strengths (R in erg·esu·cm/Gauss), $|\mu|$ (in esu-cm), $|m|$ (in erg-G^{-1}), cos θ, g_{CD}, and $|m|/|\mu|$ values of the first sixteen excited states of *trans*-(BPY)$_4$ for three conformers obtained at RI-ADC(2)/def2-TZVPD level

State	irrep	E_g	f_{osc}	$R/10^{-40}$	$\|\mu\|/10^{-20}$	$\|m\|/10^{-20}$	cos θ	g_{CD}	$\|m\|/\|\mu\|$
				***o*-**					
S_1	A	4.33	0.000	0.00	3.537	0.000	0.000	0.000	0.000
S_2	A	4.35	0.000	0.00	0.000	0.752	0.000	0.000	Inf
S_3	B	4.35	0.001	0.00	28.699	0.000	0.000	0.000	0.000
S_4	A	4.36	0.000	0.00	2.665	0.000	0.992	0.000	0.000
S_5	A	4.38	0.000	0.00	0.000	2.578	0.000	0.000	Inf
S_6	A	4.39	0.000	0.00	14.058	0.000	0.000	0.000	0.000
S_7	B	4.41	0.013	0.00	87.001	0.000	0.000	0.000	0.000
S_8	B	4.46	2.060	0.00	1104.190	0.000	0.000	0.000	0.000
S_9	A	4.46	0.000	0.00	0.000	0.881	0.000	0.000	Inf
S_{10}	A	4.51	0.009	-0.01	73.286	0.000	-0.763	0.000	0.000
S_{11}	A	4.70	0.000	0.00	10.560	0.000	0.000	0.000	0.000
S_{12}	B	4.79	0.747	0.00	641.601	0.000	0.000	0.000	0.000
S_{13}	B	4.97	0.465	0.00	497.053	0.000	0.000	0.000	0.000
S_{14}	B	5.12	0.067	0.00	186.130	0.000	0.000	0.000	0.000
S_{15}	B	5.27	0.216	0.00	328.783	0.000	0.000	0.000	0.000
S_{16}	B	5.46	1.809	0.00	934.459	0.000	0.000	0.000	0.000
				***m*-**					
S_1	B	3.82	3.796	-9.29	1619.100	0.038	-0.151	0.000	0.000
S_2	A	4.09	0.002	-1.47	34.167	0.043	-1.000	-0.005	0.001
S_3	B	4.17	0.032	-4.72	141.604	0.346	-0.096	-0.001	0.002
S_4	A	4.19	0.000	2.67	13.522	0.198	1.000	0.059	0.015
S_5	A	4.28	0.001	-4.97	18.814	0.264	-1.000	-0.056	0.014
S_6	B	4.33	0.110	13.53	258.454	0.295	0.178	0.001	0.001
S_7	A	4.50	0.000	-2.76	11.727	0.236	-1.000	-0.080	0.020
S_8	B	4.52	0.288	98.00	409.653	0.513	0.466	0.002	0.001
S_9	A	4.54	0.000	3.47	6.923	0.502	1.000	0.288	0.072
S_{10}	B	4.57	0.000	-0.14	1.240	0.372	-0.303	-0.334	0.300
S_{11}	A	4.64	0.000	4.94	14.121	0.350	1.000	0.099	0.025
S_{12}	B	4.64	0.007	11.30	60.993	0.237	0.781	0.012	0.004
S_{13}	A	4.71	0.001	-0.65	18.426	0.035	-1.000	-0.008	0.002
S_{14}	B	4.72	0.004	30.48	46.522	0.659	0.995	0.056	0.014
S_{15}	B	4.74	0.120	-252.97	258.214	1.039	-0.943	-0.015	0.004
S_{16}	A	4.76	0.001	-4.68	16.917	0.277	-1.000	-0.065	0.016
				***p*-**					
S_1	A	4.33	0.010	8.75	76.791	0.114	1.000	0.006	0.001
S_2	B	4.33	0.002	-8.61	34.083	0.340	-0.744	-0.030	0.010
S_3	A	4.37	0.000	6.06	7.753	0.782	1.000	0.399	0.101
S_4	B	4.37	0.015	-26.28	95.222	0.367	-0.752	-0.012	0.004
S_5	A	4.52	0.000	-6.77	8.720	0.777	-1.000	-0.354	0.089
S_6	B	4.52	0.152	-138.91	297.647	0.808	-0.578	-0.006	0.003
S_7	A	4.54	0.032	49.94	136.574	0.366	1.000	0.011	0.003
S_8	B	4.56	0.282	-36.31	403.326	0.735	-0.122	-0.001	0.002
S_9	A	4.61	0.008	6.04	68.041	0.089	1.000	0.005	0.001
S_{10}	B	4.61	0.013	22.63	84.615	1.256	0.213	0.013	0.015
S_{11}	B	4.63	0.795	461.84	673.165	2.235	0.307	0.004	0.003
S_{12}	A	4.63	0.094	-305.63	231.629	1.320	-1.000	-0.023	0.006
S_{13}	B	4.68	0.152	286.69	292.923	1.710	0.572	0.013	0.006
S_{14}	A	4.69	0.029	-14.02	127.547	0.110	-1.000	-0.003	0.001
S_{15}	B	4.89	0.435	549.80	484.638	4.221	0.269	0.009	0.009
S_{16}	A	4.89	0.230	-628.03	352.488	1.782	-1.000	-0.020	0.005

Table S10: E_g, f_{osc}, Rotatory Strengths (R in erg·esu·cm/Gauss), $|\mu|$ (in esu-cm), $|m|$ (in erg-G^{-1}), cos θ, g_{CD}, and $|m|/|\mu|$ values of the first sixteen excited states of *cis*-(BPY)$_4$ for three conformers obtained at RI-ADC(2)/def2-TZVPD level

State	irrep	E_g	f_{osc}	$R/10^{-40}$	$\|\mu\|/10^{-20}$	$\|m\|/10^{-20}$	cos θ	g_{CD}	$\|m\|/\|\mu\|$
				o-					
S_1	A	4.02	0.000	0.74	13.041	0.057	1.000	0.017	0.004
S_2	B	4.02	0.000	0.63	6.979	0.228	0.395	0.052	0.033
S_3	A	4.24	0.001	-1.45	22.833	0.063	-1.000	-0.011	0.003
S_4	B	4.24	0.000	-4.69	16.672	0.327	-0.861	-0.068	0.020
S_5	A	4.34	0.000	4.41	17.004	0.260	1.000	0.061	0.015
S_6	B	4.35	0.003	9.36	39.451	0.478	0.496	0.024	0.012
S_7	A	4.38	0.000	0.75	14.946	0.050	1.000	0.013	0.003
S_8	A	4.40	0.001	2.95	19.019	0.155	1.000	0.033	0.008
S_9	B	4.40	0.002	-25.55	35.812	0.729	-0.979	-0.080	0.020
S_{10}	B	4.46	0.000	-10.39	16.733	0.643	-0.966	-0.148	0.038
S_{11}	A	4.48	0.002	-25.68	33.354	0.770	-1.000	-0.092	0.023
S_{12}	B	4.49	0.005	-5.41	53.307	0.250	-0.406	-0.008	0.005
S_{13}	A	4.56	0.102	-316.42	243.441	1.300	-1.000	-0.021	0.005
S_{14}	B	4.56	0.031	368.34	134.373	3.538	0.775	0.082	0.026
S_{15}	A	4.57	0.054	-187.12	175.980	1.063	-1.000	-0.024	0.006
S_{16}	B	4.59	0.051	356.53	171.450	3.094	0.672	0.049	0.018
				m-					
S_1	B	4.08	3.128	-324.94	1422.290	1.683	-0.136	-0.001	0.001
S_2	A	4.17	0.004	-13.595	51.910	0.262	-1.000	-0.020	0.005
S_3	B	4.18	0.128	-12.36	284.552	0.449	-0.097	-0.001	0.002
S_4	A	4.28	0.005	22.26	55.848	0.399	1.000	0.029	0.007
S_5	B	4.31	0.064	19.32	198.506	0.364	0.267	0.002	0.002
S_6	A	4.37	0.007	4.46	66.594	0.067	1.000	0.004	0.001
S_7	B	4.42	0.330	284.18	443.343	0.986	0.650	0.006	0.002
S_8	A	4.48	0.038	11.45	148.589	0.077	1.000	0.002	0.001
S_9	B	4.54	0.009	38.60	70.826	0.746	0.731	0.031	0.011
S_{10}	A	4.56	0.008	-18.68	66.878	0.279	-1.000	-0.017	0.004
S_{11}	B	4.70	0.185	38.01	322.158	0.880	0.134	0.002	0.003
S_{12}	A	4.75	0.003	2.79	43.385	0.064	1.000	0.006	0.001
S_{13}	A	4.77	0.000	-0.81	2.366	0.344	-1.000	-0.569	0.145
S_{14}	B	4.77	0.000	0.81	6.045	0.345	0.387	0.088	0.057
S_{15}	B	4.77	0.124	182.06	262.179	0.766	0.906	0.011	0.003
S_{16}	A	4.79	0.011	-30.67	76.059	0.403	-1.000	-0.021	0.005
				p-					
S_1	A	4.20	0.001	4.11	29.829	0.138	1.000	0.019	0.005
S_2	B	4.20	0.004	21.21	49.720	0.802	0.532	0.034	0.016
S_3	B	4.30	0.002	0.40	34.899	0.024	0.487	0.001	0.001
S_4	A	4.31	0.001	18.05	27.545	0.655	1.000	0.095	0.024
S_5	A	4.35	0.003	28.13	43.081	0.653	1.000	0.061	0.015
S_6	B	4.35	0.017	41.20	100.048	0.816	0.505	0.017	0.008
S_7	B	4.37	0.005	19.42	53.638	0.698	0.519	0.027	0.013
S_8	A	4.42	0.001	17.96	23.023	0.780	1.000	0.135	0.034
S_9	A	4.45	0.001	-14.58	18.690	0.780	-1.000	-0.167	0.042
S_{10}	B	4.50	0.021	46.00	110.008	1.290	0.324	0.015	0.012
S_{11}	B	4.55	0.041	-18.81	153.927	1.250	-0.098	-0.003	0.008
S_{12}	A	4.65	0.173	-190.09	313.104	0.607	-1.000	-0.008	0.002
S_{13}	B	4.67	0.011	4.94	79.276	0.772	0.081	0.003	0.010
S_{14}	A	4.69	0.003	-9.37	41.180	0.227	-1.000	-0.022	0.006
S_{15}	B	4.69	0.033	-33.20	135.208	0.716	-0.343	-0.007	0.005
S_{16}	A	4.71	0.002	-6.18	30.604	0.202	-1.000	-0.026	0.007

Table S11: Excitation energies (E_g) and oscillator strengths(f_{osc}) of three different conformers for *trans*-$(BPY)_4$ calculated at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

	RI-ADC(2)			CAM-B3LYP			B3LYP		
State	Irrep	E_g	f_{osc}	Irrep	E_g	f_{osc}	Irrep	E_g	f_{osc}
o-									
S_1	A	4.33	0.000	A	4.43	0.000	A	3.89	0.000
S_2	B	4.35	0.001	B	4.43	0.064	B	3.89	0.001
S_3	A	4.35	0.000	B	4.47	1.344	A	3.96	0.000
S_4	A	4.36	0.000	B	4.49	1.060	B	3.97	0.015
S_5	A	4.38	0.000	A	4.49	0.000	A	4.07	0.000
S_6	A	4.39	0.000	A	4.55	0.000	B	4.09	0.000
S_7	B	4.41	0.013	B	4.59	0.000	A	4.10	0.000
S_8	B	4.46	2.060	A	4.59	0.002	B	4.11	1.741
S_9	A	4.46	0.000	B	4.61	0.000	B	4.11	0.026
S_{10}	A	4.51	0.009	A	4.61	0.001	A	4.12	0.000
S_{11}	A	4.70	0.000	A	4.63	0.007	B	4.13	0.000
S_{12}	B	4.79	0.747	B	4.65	0.000	A	4.13	0.000
S_{13}	B	4.97	0.465	A	4.71	0.000	A	4.17	0.000
S_{14}	B	5.12	0.067	B	4.76	0.784	B	4.17	0.000
S_{15}	B	5.27	0.216	A	4.82	0.000	A	4.23	0.006
S_{16}	B	5.46	1.809	B	4.84	0.000	A	4.25	0.000
m-									
S_1	B	3.82	3.795	B	3.75	3.723	B	3.22	2.928
S_2	A	4.09	0.002	A	4.16	0.000	A	3.65	0.000
S_3	B	4.17	0.032	A	4.38	0.003	A	3.69	0.000
S_4	A	4.19	0.000	B	4.43	0.011	A	3.75	0.001
S_5	A	4.28	0.001	A	4.50	0.001	B	3.82	0.009
S_6	B	4.33	0.110	B	4.53	0.026	A	3.94	0.000
S_7	A	4.50	0.000	B	4.55	0.273	B	4.00	0.157
S_8	B	4.52	0.288	A	4.70	0.000	B	4.01	0.527
S_9	A	4.54	0.000	A	4.74	0.001	B	4.03	0.021
S_{10}	B	4.57	0.000	B	4.75	0.001	B	4.14	0.001
S_{11}	A	4.64	0.000	A	4.79	0.000	A	4.19	0.000
S_{12}	B	4.64	0.007	B	4.84	0.004	A	4.21	0.000
S_{13}	A	4.71	0.001	A	4.87	0.001	B	4.26	0.000
S_{14}	B	4.72	0.004	B	4.88	0.014	B	4.33	0.001
S_{15}	B	4.74	0.120	B	4.90	0.005	A	4.33	0.001
S_{16}	A	4.76	0.001	A	4.91	0.000	A	4.36	0.001
p-									
S_1	A	4.33	0.010	A	4.52	0.024	A	4.01	0.017
S_2	B	4.33	0.002	B	4.52	0.239	B	4.02	0.005
S_3	B	4.37	0.015	B	4.53	0.166	B	4.04	0.036
S_4	A	4.37	0.000	A	4.53	0.003	A	4.04	0.001
S_5	A	4.52	0.000	B	4.56	1.506	B	4.11	0.129
S_6	B	4.52	0.152	A	4.63	0.161	A	4.11	0.014
S_7	A	4.54	0.032	A	4.64	0.121	A	4.12	0.026
S_8	B	4.57	0.282	B	4.64	0.041	B	4.15	0.798
S_9	B	4.61	0.013	A	4.71	0.011	B	4.17	0.011
S_{10}	A	4.61	0.008	B	4.73	0.012	A	4.20	0.048
S_{11}	B	4.63	0.795	A	4.78	0.013	A	4.25	0.001
S_{12}	A	4.63	0.094	B	4.80	0.065	B	4.28	0.042
S_{13}	B	4.68	0.152	B	4.84	0.027	B	4.31	0.088
S_{14}	A	4.69	0.029	A	4.84	0.009	A	4.31	0.030
S_{15}	B	4.89	0.435	B	4.91	0.171	B	4.37	0.112
S_{16}	A	4.89	0.230	A	4.91	0.099	A	4.38	0.000

Table S12: Excitation energies (E_g) and oscillator strengths(f_{osc}) for three different conformers of *cis*-$(BPY)_4$ calculated at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

	RI-ADC(2)			CAM-B3LYP			B3LYP		
State	Irrep	E_g	f_{osc}	Irrep	E_g	f_{osc}	Irrep	E_g	f_{osc}
				o-					
S_1	B	4.02	0.000	B	4.36	0.000	B	3.90	0.000
S_2	A	4.02	0.000	A	4.36	0.001	A	3.91	0.000
S_3	B	4.24	0.000	A	4.56	0.000	A	4.09	0.001
S_4	A	4.25	0.001	B	4.57	0.001	B	4.09	0.000
S_5	A	4.34	0.000	B	4.61	0.005	B	4.16	0.036
S_6	B	4.35	0.003	A	4.62	0.000	A	4.17	0.003
S_7	A	4.38	0.000	A	4.62	0.001	A	4.18	0.006
S_8	B	4.40	0.002	B	4.65	0.013	B	4.18	0.009
S_9	A	4.40	0.001	A	4.66	0.020	A	4.19	0.017
S_{10}	B	4.46	0.000	B	4.67	0.002	B	4.20	0.017
S_{11}	A	4.48	0.002	B	4.70	0.065	B	4.23	0.028
S_{12}	B	4.49	0.005	A	4.71	0.172	A	4.27	0.002
S_{13}	A	4.56	0.102	A	4.78	0.003	A	4.27	0.001
S_{14}	B	4.56	0.031	B	4.78	0.013	B	4.29	0.004
S_{15}	A	4.57	0.054	A	4.88	0.026	A	4.29	0.000
S_{16}	B	4.59	0.051	B	4.89	0.011	B	4.34	0.025
				m-					
S_1	B	4.08	3.128	B	4.03	3.497	B	3.50	2.670
S_2	A	4.17	0.004	A	4.37	0.050	A	3.80	0.015
S_3	B	4.18	0.128	B	4.46	0.022	B	3.87	0.015
S_4	A	4.28	0.005	A	4.47	0.005	A	3.91	0.023
S_5	B	4.31	0.064	B	4.55	0.002	A	3.99	0.000
S_6	A	4.37	0.007	A	4.57	0.007	B	3.99	0.000
S_7	B	4.42	0.330	A	4.66	0.003	A	4.01	0.007
S_8	A	4.48	0.038	B	4.67	0.077	A	4.09	0.002
S_9	B	4.54	0.009	B	4.72	0.010	B	4.11	0.005
S_{10}	A	4.56	0.008	A	4.73	0.001	B	4.19	0.094
S_{11}	B	4.70	0.185	B	4.79	0.200	A	4.20	0.000
S_{12}	A	4.75	0.003	A	4.91	0.004	B	4.23	0.546
S_{13}	B	4.77	0.000	B	4.94	0.008	B	4.28	0.009
S_{14}	A	4.77	0.000	A	4.96	0.000	B	4.37	0.005
S_{15}	B	4.77	0.124	B	4.96	0.008	A	4.48	0.005
S_{16}	A	4.80	0.011	A	4.98	0.006	B	4.48	0.028
				p-					
S_1	B	4.20	0.004	A	4.56	0.002	A	3.92	0.001
S_2	A	4.20	0.001	B	4.57	0.004	B	3.94	0.012
S_3	B	4.30	0.002	B	4.59	0.003	B	4.00	0.000
S_4	A	4.31	0.001	A	4.60	0.000	A	4.03	0.001
S_5	A	4.35	0.003	A	4.62	0.003	B	4.04	0.006
S_6	B	4.35	0.017	B	4.63	0.009	A	4.08	0.002
S_7	B	4.37	0.005	B	4.64	0.024	B	4.08	0.002
S_8	A	4.42	0.001	A	4.66	0.007	B	4.13	0.013
S_9	A	4.45	0.001	A	4.69	0.001	A	4.13	0.003
S_{10}	B	4.50	0.021	B	4.72	0.003	B	4.15	0.006
S_{11}	B	4.55	0.041	B	4.78	0.085	A	4.15	0.001
S_{12}	A	4.65	0.173	A	4.86	0.264	A	4.17	0.001
S_{13}	B	4.67	0.011	B	4.92	0.041	B	4.25	0.005
S_{14}	A	4.69	0.003	A	4.97	0.029	B	4.29	0.002
S_{15}	B	4.70	0.033	B	5.01	0.004	A	4.32	0.103
S_{16}	A	4.71	0.002	A	5.01	0.008	A	4.34	0.000

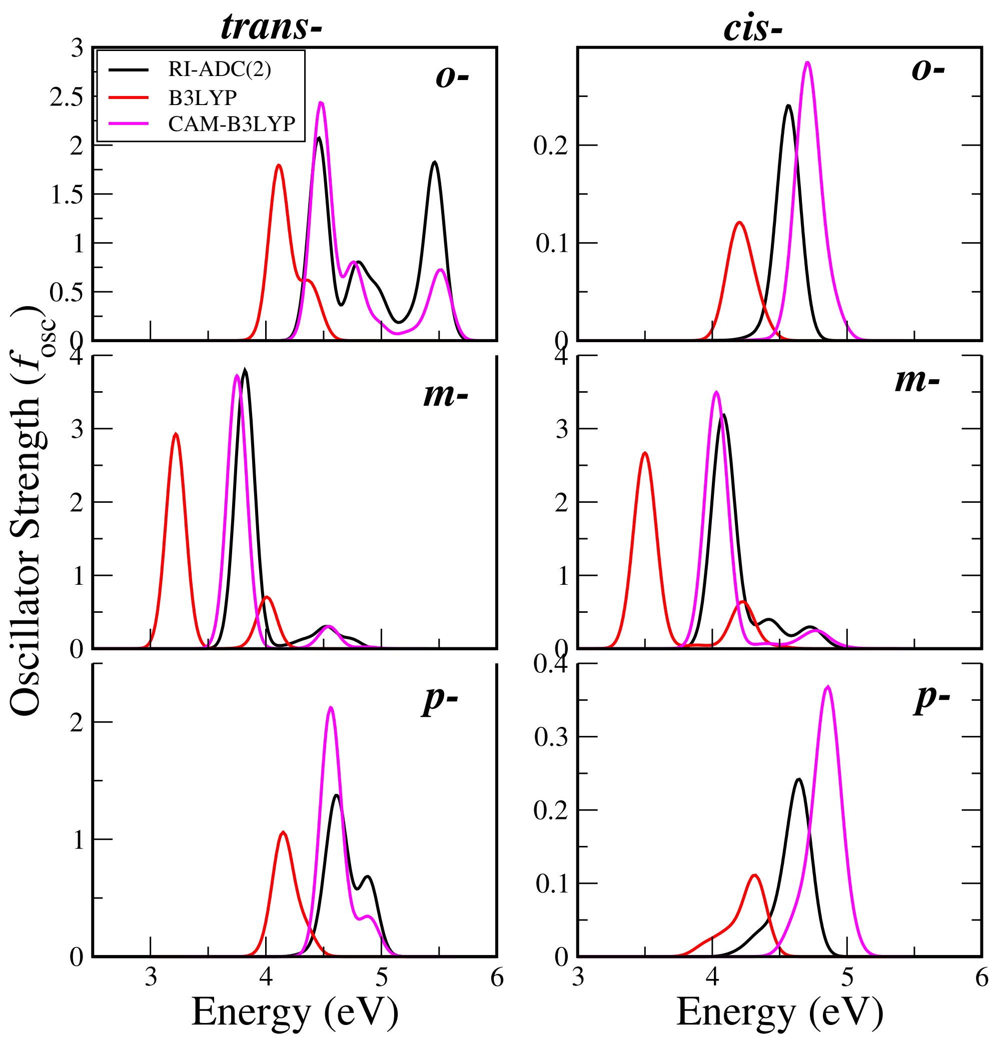

Figure S3: Absorption spectra of ***o-***, ***m-***, and ***p-*** conformers for ***trans***- and ***cis***-**(BPY)**$_4$ obtained at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

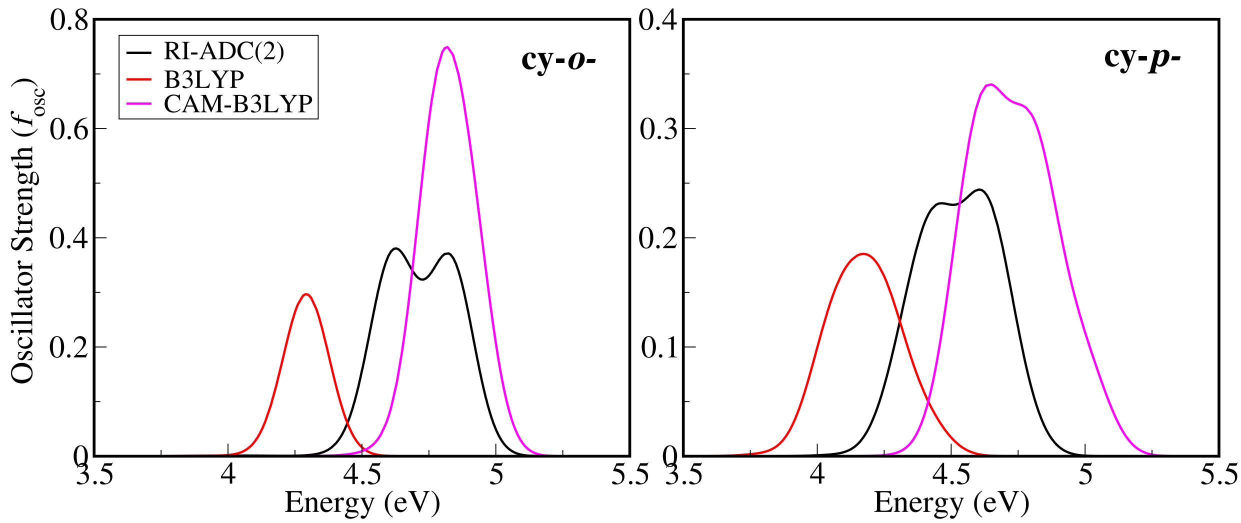

Figure S4: Absorption spectra of cy-***o*-** and cy-***p*-** obtained at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

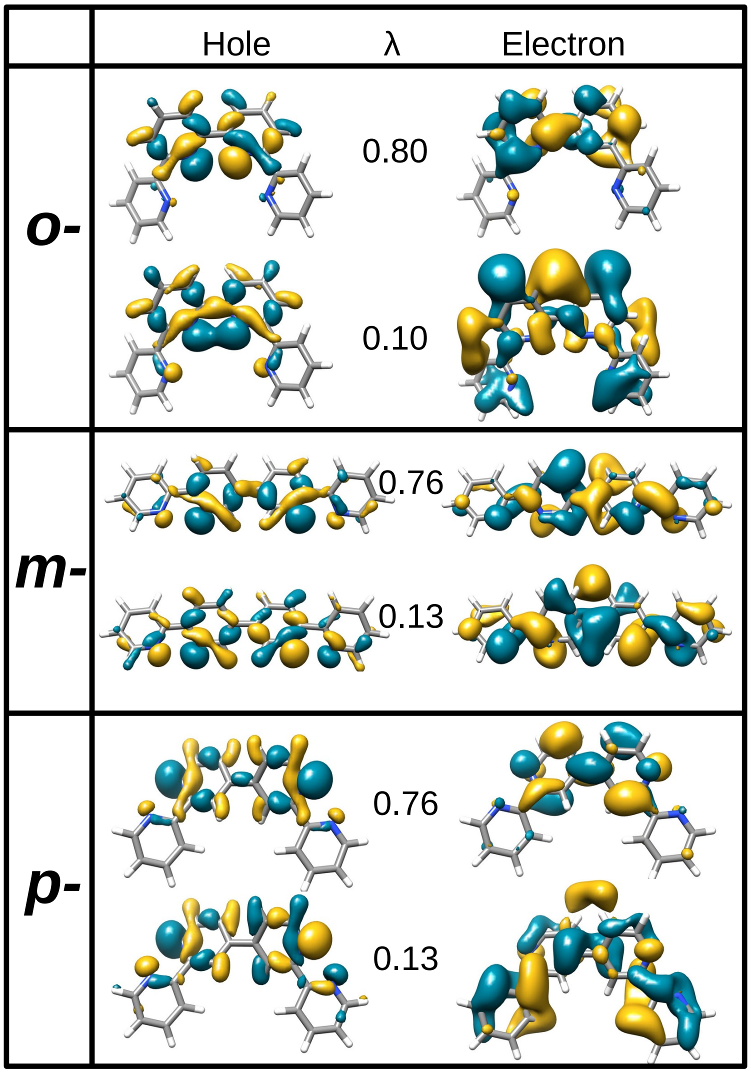

Figure S5: Natural transition orbitals corresponding to the S_1 states of three different conformers of ***cis*-(BPY)**$_2$. Here, λ value represents the weight of a configuration.

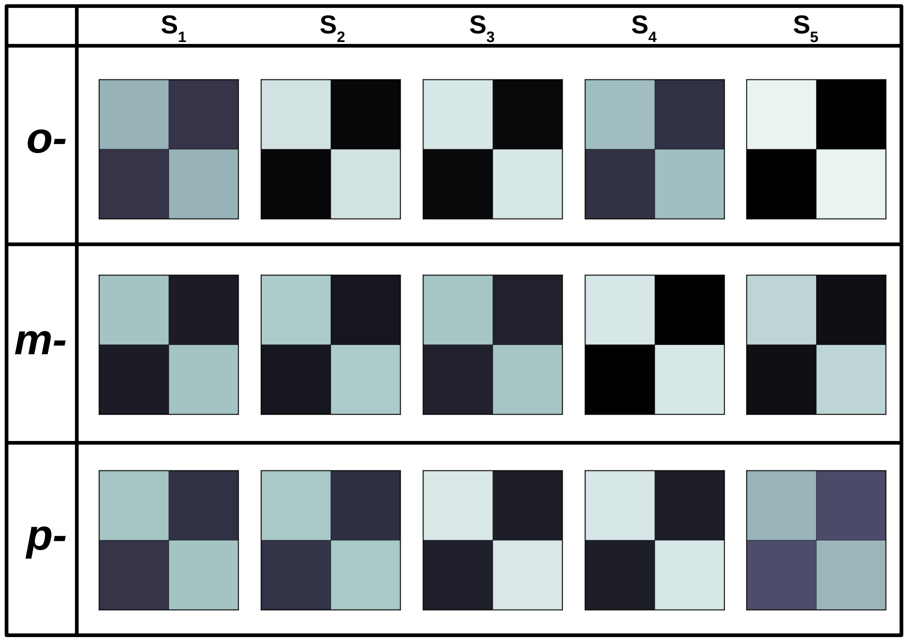

Figure S6: *e*-*h* correlation plots corresponding to the first five excited states of ***cis*-(BPY)**$_2$ for three different conformers.

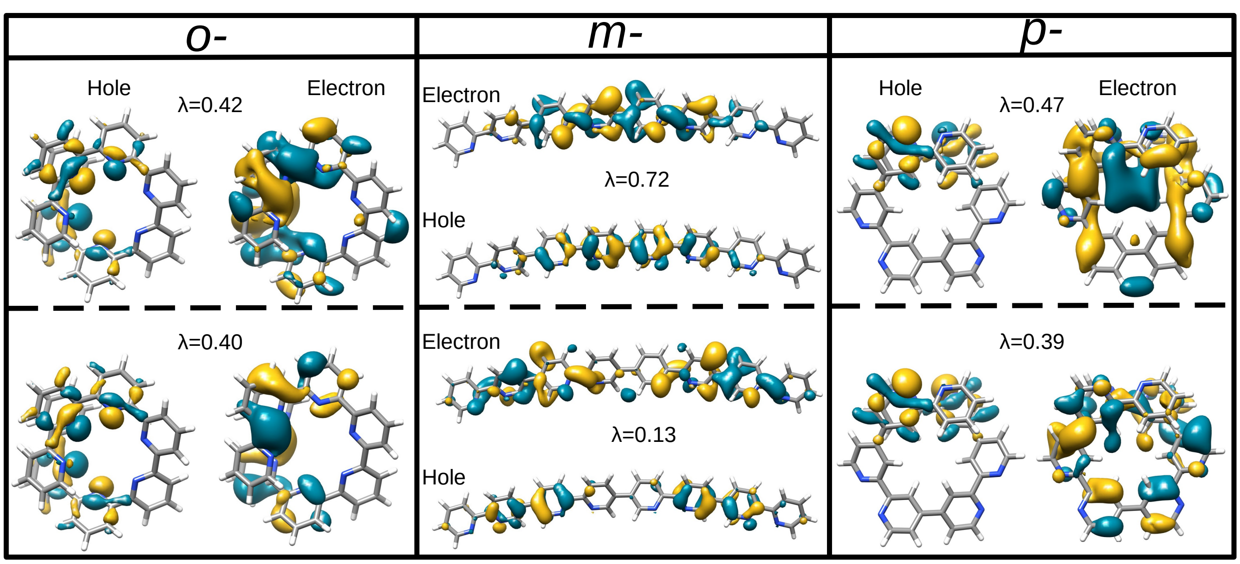

Figure S7: Natural transition orbitals corresponding to the S_1 states of three different conformers of ***cis*-(BPY)**$_4$. Here, λ value represents the weight of a configuration.

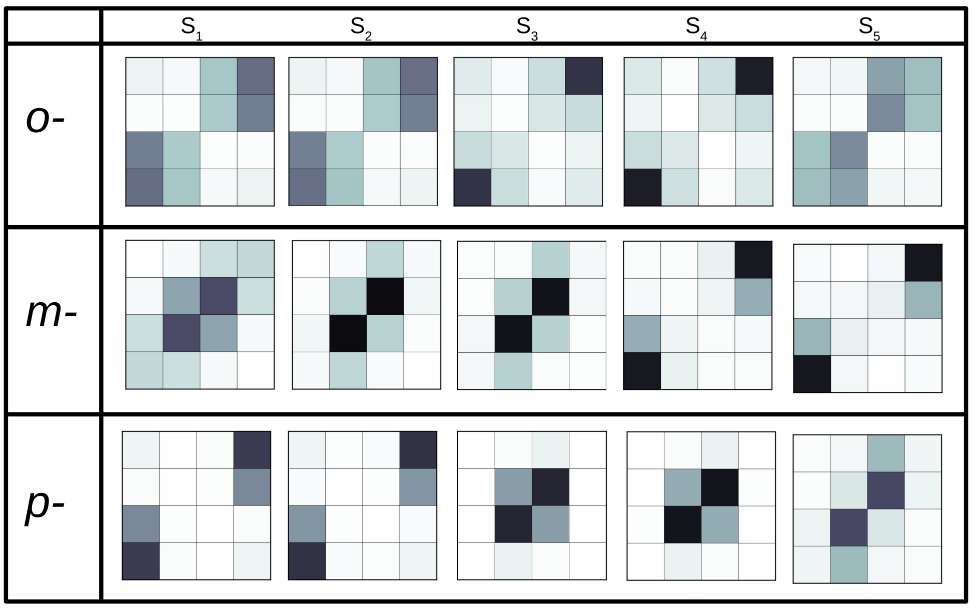

Figure S8: *e*-*h* correlation plots corresponding to the first five excited states of ***cis*-(BPY)**$_4$ for three different conformers.

Table S13: Excitation energies (E_g), oscillator strengths(f_{osc}), and ω_{CT} values of first five states of three different conformers of *trans*-(BPY)$_4$ calculated at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

					o-				
	RI-ADC(2)			CAM-B3LYP			B3LYP		
State	E_g	f_{osc}	ω_{CT}	E_g	f_{osc}	ω_{CT}	E_g	f_{osc}	ω_{CT}
S_1	4.33	0.000	0.33	4.43	0.000	0.25	3.89	0.000	0.60
S_2	4.35	0.001	0.44	4.43	0.064	0.35	3.89	0.001	0.58
S_3	4.35	0.000	0.41	4.47	1.344	0.25	3.96	0.000	0.56
S_4	4.36	0.000	0.33	4.49	1.060	0.27	3.97	0.015	0.55
S_5	4.38	0.000	0.42	4.49	0.000	0.33	4.07	0.000	0.53
					m-				
S_1	3.82	3.795	0.44	3.75	3.723	0.38	3.22	2.928	0.60
S_2	4.09	0.002	0.30	4.16	0.000	0.34	3.65	0.000	0.69
S_3	4.17	0.032	0.27	4.38	0.003	0.17	3.69	0.000	0.76
S_4	4.19	0.000	0.38	4.43	0.011	0.14	3.75	0.001	0.38
S_5	4.28	0.001	0.29	4.50	0.001	0.10	3.82	0.009	0.36
					p-				
S_1	4.33	0.010	0.19	4.52	0.024	0.11	4.01	0.017	0.25
S_2	4.33	0.002	0.19	4.52	0.239	0.10	4.02	0.005	0.24
S_3	4.37	0.015	0.19	4.53	0.166	0.09	4.04	0.036	0.20
S_4	4.37	0.000	0.18	4.53	0.003	0.08	4.04	0.001	0.19
S_5	4.52	0.000	0.47	4.56	1.506	0.12	4.11	0.129	0.51

Table S14: Excitation energies (E_g), oscillator strengths(f_{osc}), and ω_{CT} values of first five states of three different conformers of *cis*-(BPY)$_4$ calculated at RI-ADC(2) level and using two different functionals B3LYP and CAM-B3LYP using the def2-TZVPD basis set

	RI-ADC(2)			CAM-B3LYP			B3LYP		
State	E_g	f_{osc}	ω_{CT}	E_g	f_{osc}	ω_{CT}	E_g	f_{osc}	ω_{CT}
o-									
S_1	4.02	0.000	0.52	4.36	0.000	0.30	3.90	0.000	0.42
S_2	4.02	0.000	0.53	4.36	0.001	0.30	3.91	0.000	0.42
S_3	4.24	0.000	0.36	4.56	0.000	0.10	4.09	0.001	0.17
S_4	4.25	0.001	0.33	4.57	0.001	0.10	4.09	0.000	0.15
S_5	4.34	0.000	0.51	4.61	0.005	0.19	4.16	0.036	0.49
m-									
S_1	4.08	3.128	0.46	4.03	3.497	0.38	3.50	2.670	0.57
S_2	4.17	0.004	0.33	4.37	0.050	0.30	3.80	0.015	0.48
S_3	4.18	0.128	0.34	4.46	0.022	0.16	3.87	0.015	0.32
S_4	4.28	0.005	0.34	4.47	0.005	0.17	3.91	0.023	0.46
S_5	4.31	0.064	0.32	4.55	0.002	0.11	3.99	0.000	0.77
p-									
S_1	4.20	0.004	0.42	4.56	0.002	0.18	3.92	0.001	0.72
S_2	4.20	0.001	0.40	4.57	0.004	0.18	3.94	0.012	0.88
S_3	4.30	0.002	0.36	4.59	0.003	0.17	4.00	0.000	0.43
S_4	4.31	0.001	0.32	4.60	0.000	0.20	4.03	0.001	0.36
S_5	4.35	0.003	0.42	4.62	0.003	0.28	4.04	0.006	0.41

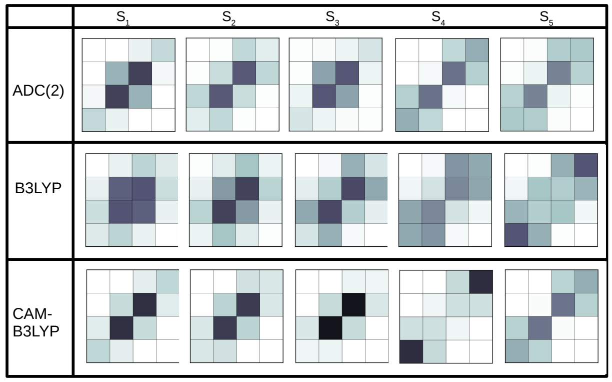

Figure S9: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***o*-*trans*-(BPY)**$_4$

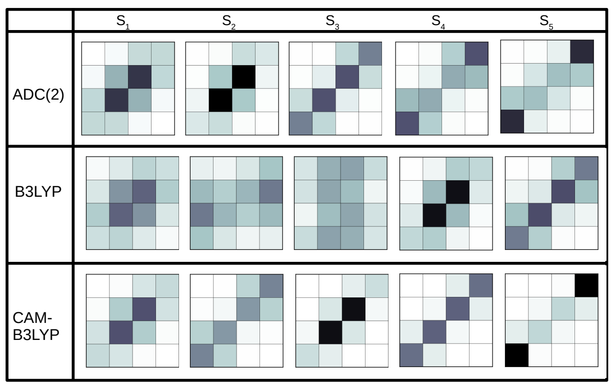

Figure S10: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***m*-*trans*-(BPY)**$_4$

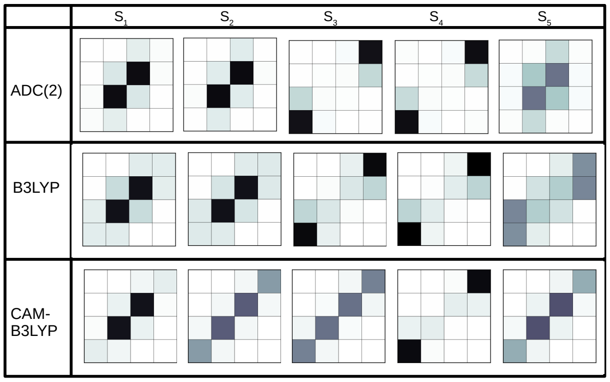

Figure S11: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***p*-*trans*-(BPY)**$_4$

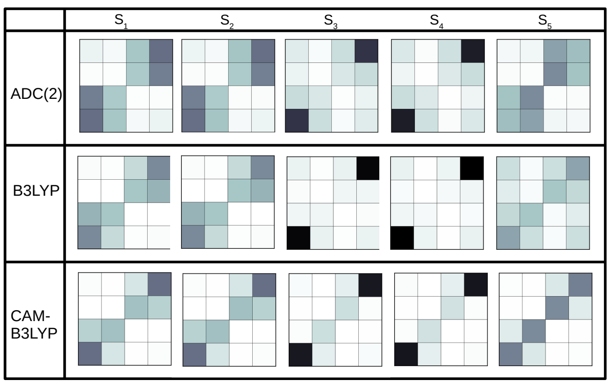

Figure S12: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***o*-*cis*-(BPY)**$_4$

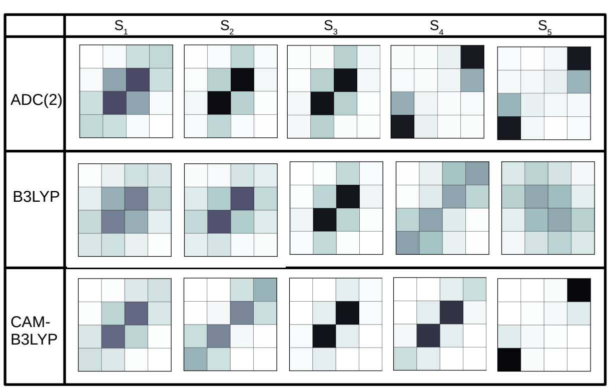

Figure S13: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***m*-*cis*-(BPY)**$_4$

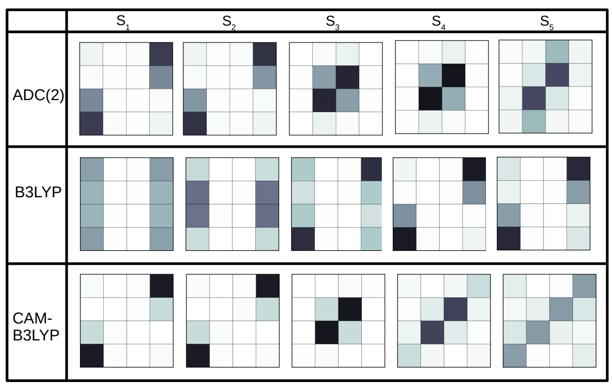

Figure S14: *e*-*h* correlation plots obtained using the RI-ADC(2) method, and B3LYP and CAM-B3LYP functionals for the first five excited states of ***p-cis*-(BPY)**$_4$