Supporting Information: Identification of receiver triplet state in the ultrafast intersystem crossing of carbonylpyrenes

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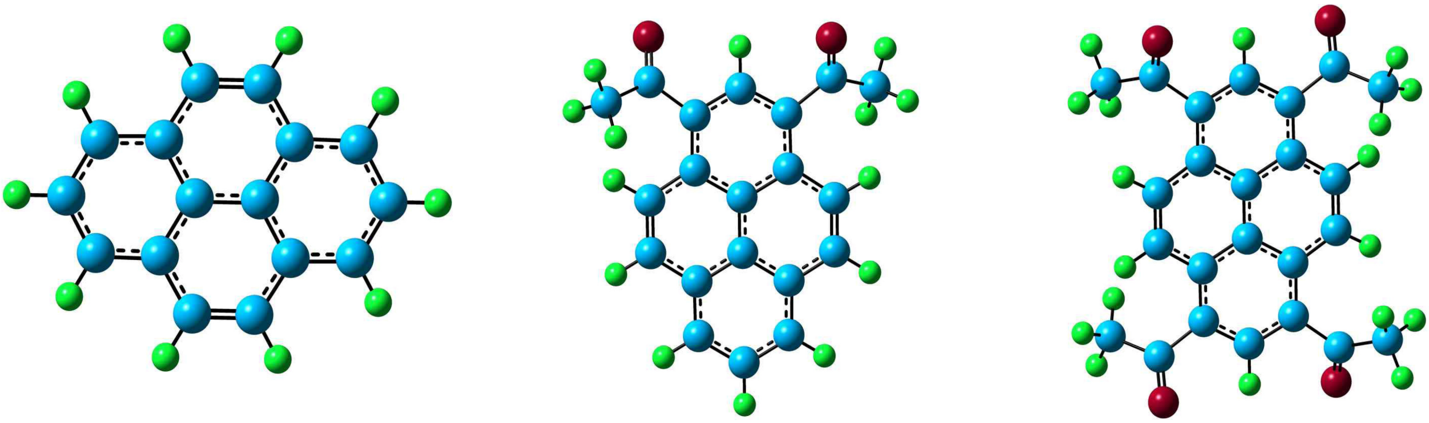

Table S1: Numbering, symmetry and harmonic frequency components of vibrational modes of **P** calculated at B3LYP/6-311G(d,p) level of theory.

No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})
ν_1 (B3U)	98.4254	ν_{26} (B1U)	834.4631	ν_{51} (AG)	1427.4565
ν_2 (AU)	152.2882	ν_{27} (B2G)	846.6147	ν_{52} (B3G)	1434.2661
ν_3 (B3U)	214.0022	ν_{28} (B3U)	859.3325	ν_{53} (B2U)	1457.8068
ν_4 (B1G)	249.3383	ν_{29} (AU)	902.4360	ν_{54} (B1U)	1459.4816
ν_5 (B2G)	262.5502	ν_{30} (B1G)	916.2475	ν_{55} (B1U)	1483.2710
ν_6 (B2U)	359.4307	ν_{31} (B2G)	973.5891	ν_{56} (B2U)	1515.5531
ν_7 (AU)	402.0617	ν_{32} (AU)	979.8860	ν_{57} (B3G)	1535.7080
ν_8 (AG)	412.1204	ν_{33} (B2U)	980.8016	ν_{58} (AG)	1596.4104
ν_9 (B3G)	462.6067	ν_{34} (B3U)	982.0027	ν_{59} (B3G)	1626.0974
ν_{10} (B3U)	500.4332	ν_{35} (B2G)	990.9897	ν_{60} (B1U)	1635.8261
ν_{11} (B1U)	507.1292	ν_{36} (B1U)	1014.9363	ν_{61} (B2U)	1645.9468
ν_{12} (B3G)	508.6963	ν_{37} (AG)	1091.2967	ν_{62} (AG)	1670.7893
ν_{13} (B2G)	513.5979	ν_{38} (B1U)	1113.9498	ν_{63} (B1U)	3155.9250
ν_{14} (B1G)	538.5187	ν_{39} (B3G)	1127.0684	ν_{64} (B3G)	3156.1961
ν_{15} (B2U)	554.2838	ν_{40} (B2U)	1165.3839	ν_{65} (AG)	3159.4343
ν_{16} (B2G)	585.9834	ν_{41} (AG)	1168.0821	ν_{66} (B1U)	3160.0565
ν_{17} (AG)	595.4396	ν_{42} (B3G)	1198.3135	ν_{67} (B2U)	3167.1859
ν_{18} (AU)	687.8000	ν_{43} (B2U)	1204.3742	ν_{68} (B3G)	3168.1101
ν_{19} (B1U)	704.0640	ν_{44} (B2U)	1232.1106	ν_{69} (AG)	3175.3078
ν_{20} (B3U)	726.2456	ν_{45} (AG)	1262.6535	ν_{70} (B2U)	3175.4013
ν_{21} (B3G)	749.5580	ν_{46} (B3G)	1264.1479	ν_{71} (B1U)	3184.2757
ν_{22} (B3U)	756.9113	ν_{47} (B1U)	1268.3282	ν_{72} (AG)	3184.7420
ν_{23} (B2G)	783.5288	ν_{48} (B2U)	1342.7285		
ν_{24} (B1G)	814.6937	ν_{49} (AG)	1351.6222		
ν_{25} (AG)	814.8641	ν_{50} (B3G)	1399.9811		

Table S2: Numbering, symmetry and harmonic frequency components of vibrational modes of **AP2** calculated at B3LYP/6-311G(d,p) level of theory.

No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})
ν_1 (A)	48.3148	ν_{39} (B)	831.0852	ν_{77} (B)	1483.3132
ν_2 (B)	50.0960	ν_{40} (A)	831.6901	ν_{78} (A)	1483.6930
ν_3 (A)	61.9289	ν_{41} (B)	842.9225	ν_{79} (A)	1490.0655
ν_4 (B)	64.8000	ν_{42} (B)	856.5355	ν_{80} (B)	1516.6380
ν_5 (B)	125.4629	ν_{43} (A)	866.5097	ν_{81} (B)	1540.1034
ν_6 (A)	145.8265	ν_{44} (A)	917.8238	ν_{82} (A)	1553.6222
ν_7 (A)	168.1223	ν_{45} (B)	951.6314	ν_{83} (B)	1615.6819
ν_8 (B)	172.3892	ν_{46} (A)	975.9206	ν_{84} (A)	1622.5586
ν_9 (B)	174.8179	ν_{47} (B)	980.9398	ν_{85} (B)	1645.7144
ν_{10} (A)	188.2988	ν_{48} (A)	987.0584	ν_{86} (A)	1665.3875
ν_{11} (B)	229.9050	ν_{49} (B)	992.9056	ν_{87} (B)	1751.7380
ν_{12} (A)	266.8663	ν_{50} (B)	999.1643	ν_{88} (A)	1755.4813
ν_{13} (B)	270.7871	ν_{51} (B)	1018.7982	ν_{89} (B)	3036.6912
ν_{14} (B)	300.2219	ν_{52} (A)	1034.3376	ν_{90} (A)	3036.7128
ν_{15} (A)	309.2736	ν_{53} (B)	1039.3946	ν_{91} (A)	3102.8402
ν_{16} (B)	345.9302	ν_{54} (A)	1060.1760	ν_{92} (B)	3102.8485
ν_{17} (A)	365.4432	ν_{55} (A)	1104.3420	ν_{93} (B)	3136.4318
ν_{18} (A)	424.3614	ν_{56} (B)	1133.0530	ν_{94} (A)	3136.4834
ν_{19} (B)	433.6336	ν_{57} (A)	1166.5286	ν_{95} (A)	3163.3564
ν_{20} (A)	484.4566	ν_{58} (B)	1185.6324	ν_{96} (B)	3167.2804
ν_{21} (B)	490.8965	ν_{59} (A)	1193.3055	ν_{97} (A)	3168.8131
ν_{22} (B)	508.7036	ν_{60} (B)	1199.9434	ν_{98} (B)	3171.7997
ν_{23} (B)	511.9942	ν_{61} (B)	1211.6843	ν_{99} (A)	3188.7418
ν_{24} (A)	533.3391	ν_{62} (B)	1242.8887	ν_{100} (A)	3212.5049
ν_{25} (B)	534.2843	ν_{63} (B)	1254.9136	ν_{101} (B)	3225.1673
ν_{26} (A)	555.8849	ν_{64} (A)	1269.1920	ν_{102} (A)	3225.2893
ν_{27} (B)	564.1284	ν_{65} (A)	1277.3792		
ν_{28} (A)	590.8234	ν_{66} (B)	1338.3130		
ν_{29} (B)	626.9759	ν_{67} (A)	1366.6826		
ν_{30} (A)	647.1956	ν_{68} (A)	1385.5320		
ν_{31} (B)	653.2707	ν_{69} (B)	1386.2529		
ν_{32} (A)	663.0799	ν_{70} (A)	1393.2832		
ν_{33} (B)	707.1562	ν_{71} (B)	1395.0052		
ν_{34} (A)	707.7125	ν_{72} (B)	1412.6582		
ν_{35} (A)	719.1865	ν_{73} (A)	1443.8934		
ν_{36} (B)	733.7522	ν_{74} (B)	1446.2475		
ν_{37} (B)	771.4456	ν_{75} (B)	1474.7533		
ν_{38} (A)	827.2436	ν_{76} (A)	1474.8586		

Table S3: Numbering, symmetry and harmonic frequency components of vibrational modes of **AP4** calculated at B3LYP/6-311G(d,p) level of theory.

No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})	No.(Sym.)	Freq (in cm^{-1})
ν_{1} (AU)	30.2273	ν_{54} (AU)	832.5737	ν_{107} (AU)	1589.6381
ν_{2} (BU)	40.3238	ν_{55} (AG)	837.5251	ν_{108} (BG)	1606.0219
ν_{3} (AG)	52.1607	ν_{56} (BU)	843.5187	ν_{109} (BU)	1646.8165
ν_{4} (BG)	52.3407	ν_{57} (BG)	885.9474	ν_{110} (AG)	1659.2871
ν_{5} (BU)	54.4024	ν_{58} (AG)	929.0344	ν_{111} (BG)	1755.7936
ν_{6} (AU)	56.7593	ν_{59} (BU)	946.8030	ν_{112} (BU)	1755.9127
ν_{7} (AG)	78.8058	ν_{60} (BG)	963.3721	ν_{113} (AU)	1757.5353
ν_{8} (BG)	103.1405	ν_{61} (AU)	976.2488	ν_{114} (AG)	1761.0436
ν_{9} (BU)	105.8821	ν_{62} (AG)	985.6325	ν_{115} (BG)	3037.7042
ν_{10} (AG)	144.4761	ν_{63} (BG)	990.3140	ν_{116} (AU)	3037.7242
ν_{11} (AU)	151.4541	ν_{64} (AU)	992.0594	ν_{117} (BU)	3037.7642
ν_{12} (BU)	153.4361	ν_{65} (BU)	1000.1593	ν_{118} (AG)	3037.7848
ν_{13} (AU)	167.1370	ν_{66} (BG)	1007.3150	ν_{119} (AU)	3103.5618
ν_{14} (BG)	167.1537	ν_{67} (AU)	1034.1337	ν_{120} (BG)	3103.5671
ν_{15} (AG)	171.2940	ν_{68} (BU)	1034.5790	ν_{121} (AG)	3103.6209
ν_{16} (BU)	174.6969	ν_{69} (AG)	1036.0336	ν_{122} (BU)	3103.6311
ν_{17} (BG)	194.9366	ν_{70} (BU)	1038.2146	ν_{123} (BG)	3137.3281
ν_{18} (AU)	209.5500	ν_{71} (BG)	1039.3412	ν_{124} (AU)	3137.3443
ν_{19} (BU)	241.3192	ν_{72} (AU)	1080.1457	ν_{125} (BU)	3137.3971
ν_{20} (AG)	272.5689	ν_{73} (AG)	1133.4944	ν_{126} (AG)	3137.4775
ν_{21} (BG)	276.2921	ν_{74} (BG)	1138.6556	ν_{127} (AU)	3212.9428
ν_{22} (AG)	276.4776	ν_{75} (BU)	1200.7678	ν_{128} (AG)	3213.0611
ν_{23} (BG)	304.7693	ν_{76} (BG)	1203.0145	ν_{129} (BG)	3213.4032
ν_{24} (BU)	317.3768	ν_{77} (AG)	1207.4304	ν_{130} (AU)	3213.4431
ν_{25} (AU)	330.4686	ν_{78} (AU)	1214.4213	ν_{131} (BU)	3229.9576
ν_{26} (BU)	348.0975	ν_{79} (BU)	1216.2391	ν_{132} (BU)	3230.0883
ν_{27} (AU)	379.6583	ν_{80} (BU)	1245.4556		
ν_{28} (BG)	380.3656	ν_{81} (BG)	1249.1632		
ν_{29} (AG)	388.7587	ν_{82} (AG)	1275.8627		
ν_{30} (BU)	462.9933	ν_{83} (AU)	1284.1516		
ν_{31} (AU)	491.5166	ν_{84} (BU)	1337.1036		
ν_{32} (AG)	499.8981	ν_{85} (AG)	1369.1968		
ν_{33} (BG)	509.3557	ν_{86} (AG)	1385.4120		
ν_{34} (BG)	525.6432	ν_{87} (BG)	1385.9199		
ν_{35} (BU)	531.0913	ν_{88} (AU)	1387.3990		
ν_{36} (BG)	542.9742	ν_{89} (BG)	1387.4350		
ν_{37} (AG)	554.4809	ν_{90} (BU)	1388.4439		
ν_{38} (AU)	574.2593	ν_{91} (AG)	1389.8790		
ν_{39} (BG)	589.2751	ν_{92} (BU)	1394.1417		
ν_{40} (AG)	591.2928	ν_{93} (AU)	1410.5284		
ν_{41} (BU)	612.3613	ν_{94} (BG)	1431.9675		
ν_{42} (AU)	616.1313	ν_{95} (BG)	1473.9667		
ν_{43} (AU)	655.9481	ν_{96} (AU)	1474.2320		
ν_{44} (BU)	658.9983	ν_{97} (BU)	1475.3306		
ν_{45} (AG)	669.7171	ν_{98} (AG)	1475.6384		
ν_{46} (BG)	679.2529	ν_{99} (AU)	1483.8964		
ν_{47} (AG)	680.3140	ν_{100} (BG)	1484.1027		
ν_{48} (AU)	710.6873	ν_{101} (BU)	1484.1510		
ν_{49} (BG)	712.0282	ν_{102} (AG)	1485.1042		
ν_{50} (AU)	733.4121	ν_{103} (AU)	1492.7456		
ν_{51} (BU)	733.8512	ν_{104} (BU)	1522.8208		
ν_{52} (BU)	760.8984	ν_{105} (AG)	1533.0119		
ν_{53} (BG)	817.1631	ν_{106} (BG)	1538.7536		

Table S4: VEE (in eV) of **P, AP2** & **AP4** obtained at B3LYP/6-311G(d,p) level of theory. Oscillator strength shown in paranthesis.

	P	**AP2**	**AP4**		**P**	**AP2**	**AP4**
S_1	3.6924 (0.2537)	3.2633 (0.3646)	3.0198 (0.4607)	T_1	2.1580	1.9434	1.7892
S_2	3.7576 (0.0002)	3.3499 (0.0106)	3.0899 (0.0235)	T_2	3.4459	2.9345	2.6941
S_3	4.3744 (0.0000)	3.5743 (0.0181)	3.2234 (0.0000)	T_3	3.5684	3.1456	2.8945
S_4	4.6016 (0.2648)	3.5784 (0.0014)	3.3917 (0.0000)	T_4	3.5920	3.2336	3.0049
S_5	4.6249 (0.0000)	4.0956 (0.0470)	3.3945 (0.0479)	T_5	3.8952	3.4517	3.0397
S_6	5.0539 (0.0000)	4.2718 (0.1104)	3.4398 (0.0113)	T_6	3.8969	3.5152	3.0921

Table S5: Vibronic Hamiltonian matrices (H') constructed for the singlet and triplet manifold of **P, AP2** & **AP4.**

Singlets:

P, **AP2** & **AP4**:

$$H' = \begin{pmatrix} E_{S_1}^{(0)} + \sum_t \kappa_t^{(S_1)} Q_t & \sum_{nt} \lambda_{nt}^{(12)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(13)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(14)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(15)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(16)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(21)} Q_{nt} & E_{S_2}^{(0)} + \sum_t \kappa_t^{(S_2)} Q_t & \sum_{nt} \lambda_{nt}^{(23)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(24)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(25)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(26)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(31)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(32)} Q_{nt} & E_{S_3}^{(0)} + \sum_t \kappa_t^{(S_3)} Q_t & \sum_{nt} \lambda_{nt}^{(34)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(35)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(36)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(41)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(42)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(43)} Q_{nt} & E_{S_4}^{(0)} + \sum_t \kappa_t^{(S_4)} Q_t & \sum_{nt} \lambda_{nt}^{(45)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(46)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(51)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(52)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(53)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(54)} Q_{nt} & E_{S_5}^{(0)} + \sum_t \kappa_t^{(S_5)} Q_t & \sum_{nt} \lambda_{nt}^{(56)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(61)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(62)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(63)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(64)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(65)} Q_{nt} & E_{S_6}^{(0)} + \sum_t \kappa_t^{(S_6)} Q_t \end{pmatrix}$$

Triplets:

P & **AP2**:

$$H' = \begin{pmatrix} E_{T_1}^{(0)} + \sum_t \kappa_t^{(T_1)} Q_t & \sum_{nt} \lambda_{nt}^{(12)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(13)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(14)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(21)} Q_{nt} & E_{T_2}^{(0)} + \sum_t \kappa_t^{(T_2)} Q_t & \sum_{nt} \lambda_{nt}^{(23)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(24)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(31)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(32)} Q_{nt} & E_{T_3}^{(0)} + \sum_t \kappa_t^{(T_3)} Q_t & \sum_{nt} \lambda_{nt}^{(34)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(41)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(42)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(43)} Q_{nt} & E_{T_4}^{(0)} + \sum_t \kappa_t^{(T_4)} Q_t \end{pmatrix}$$

AP4:

$$H' = \begin{pmatrix} E_{T_1}^{(0)} + \sum_t \kappa_t^{(T_1)} Q_t & \sum_{nt} \lambda_{nt}^{(12)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(13)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(14)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(15)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(21)} Q_{nt} & E_{T_2}^{(0)} + \sum_t \kappa_t^{(T_2)} Q_t & \sum_{nt} \lambda_{nt}^{(23)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(24)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(25)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(31)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(32)} Q_{nt} & E_{T_3}^{(0)} + \sum_t \kappa_t^{(T_3)} Q_t & \sum_{nt} \lambda_{nt}^{(34)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(35)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(41)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(42)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(43)} Q_{nt} & E_{T_4}^{(0)} + \sum_t \kappa_t^{(T_4)} Q_t & \sum_{nt} \lambda_{nt}^{(45)} Q_{nt} \\ \sum_{nt} \lambda_{nt}^{(51)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(52)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(53)} Q_{nt} & \sum_{nt} \lambda_{nt}^{(54)} Q_{nt} & E_{T_5}^{(0)} + \sum_t \kappa_t^{(T_5)} Q_t \end{pmatrix}$$

Table S6: Linear intrastate coupling parameters (κ) for singlet electronic states of **P** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

AG mode (Freq, eV)	κ^{S_1}	κ^{S_2}	κ^{S_3}	κ^{S_4}	κ^{S_5}	κ^{S_6}
ν_8(0.0511)	-0.0363(0.2523)	-0.0108(0.0223)	-0.0226(0.0978)	-0.0165(0.0524)	-0.0902(1.5592)	-0.0261(0.1305)
ν_{17}(0.0738)	-0.0151(0.0209)	-0.0359(0.1183)	-0.0163(0.0245)	-0.0396(0.1442)	-0.0310(0.0885)	-0.0434(0.1726)
ν_{25}(0.1010)	-0.0088(0.0038)	-0.0029(0.0004)	-0.0006(0.0001)	-0.0051(0.0013)	-0.0771(0.2914)	0.0203(0.0202)
ν_{37}(0.1353)	-0.0165(0.0074)	-0.0475(0.0616)	-0.0130(0.0046)	-0.0450(0.0554)	0.0169(0.0078)	-0.0242(0.0160)
ν_{41}(0.1448)	-0.0333(0.0264)	0.0115(0.0032)	-0.0735 (0.1289)	-0.0007(0.0001)	-0.0434(0.0450)	-0.0448(0.0478)
ν_{45}(0.1565)	0.1123(0.2575)	0.0883(0.1592)	0.0453(0.0420)	0.0640(0.0837)	0.0501(0.0513)	0.0791(0.1277)
ν_{49}(0.1676)	-0.0086(0.0013)	-0.0234(0.0097)	-0.0512(0.0467)	-0.0185(0.0061)	-0.1039(0.1923)	0.0598(0.0637)
ν_{51}(0.1770)	-0.1037(0.1716)	-0.1212(0.2344)	-0.0084(0.0011)	-0.0880(0.1235)	-0.0309(0.0152)	-0.0248(0.0098)
ν_{58}(0.1979)	-0.0068(0.0006)	0.0559(0.0399)	0.0576(0.0424)	0.0534(0.0364)	0.0138(0.0024)	-0.0367(0.0172)
ν_{62}(0.2072)	0.1486(0.2572)	-0.0127(0.0019)	0.2721(0.8625)	0.0101(0.0012)	0.2202(0.5645)	0.1334(0.2074)
ν_{65}(0.3917)	-0.0054(0.0001)	0.0009(0.0001)	0.0006(0.0001)	-0.0008(0.0001)	-0.0130(0.0005)	-0.0122(0.0005)
ν_{69}(0.3937)	-0.0080(0.0002)	-0.0025(0.0001)	-0.0223(0.0016)	-0.0046(0.0001)	-0.0119(0.0005)	-0.0088(0.0002)
ν_{72}(0.3949)	0.0096(0.0003)	0.0164(0.0009)	0.0108(0.0004)	0.0154(0.0008)	0.0084(0.0002)	0.0138(0.0006)

Table S7: Linear interstate coupling parameters (λ) for singlet electronic states of **P** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

Vibrational mode (Freq, eV)	$\lambda_{S_1-S_2}$	$\lambda_{S_1-S_3}$	$\lambda_{S_1-S_4}$	$\lambda_{S_1-S_5}$	$\lambda_{S_1-S_6}$	$\lambda_{S_2-S_3}$	$\lambda_{S_2-S_5}$	$\lambda_{S_2-S_6}$	$\lambda_{S_3-S_4}$	$\lambda_{S_3-S_6}$	$\lambda_{S_4-S_5}$	$\lambda_{S_4-S_6}$	$\lambda_{S_5-S_6}$
ν_6(0.0446)	-	0.0267(0.1792)	-	0.0284(0.2027)	-	-	-	-	-	-	-	-	-
ν_9(0.0574)	0.0090(0.0123)	-	0.0346(0.1817)	-	-	-	-	-	-	0.0401(0.2440)	-	-	0.0344(0.1796)
ν_{11}(0.0629)	-	-	-	-	0.0045(0.0026)	-	0.0305(0.1176)	-	-	-	0.0053(0.0035)	-	-
ν_{12}(0.0631)	0.0081(0.0082)	-	0.0328(0.1351)	-	-	-	-	-	-	0.0164(0.0338)	-	-	0.0139(0.0243)
ν_{15}(0.0687)	-	0.0473(0.2370)	-	0.0555(0.3263)	-	-	-	-	-	-	-	0.0305(0.0985)	-
ν_{19}(0.0873)	-	-	-	-	0.0159(0.0166)	0.0276(0.0500)	0.1221(0.9781)	-	-	-	0.0369(0.0893)	-	-
ν_{21}(0.0929)	0.0070(0.0028)	-	0.0224(0.0291)	-	-	-	-	-	-	0.0090(0.0047)	-	-	-
ν_{26}(0.1035)	-	-	-	-	0.0267(0.0333)	-	0.1131(0.5971)	-	-	-	0.0355(0.0588)	-	-
ν_{33}(0.1216)	-	0.0160(0.0087)	-		-	-	-	0.0112(0.0042)	-	-	-	0.0150(0.0076)	-
ν_{36}(0.1258)	-	-	-	-	0.0218(0.0150)	0.0327(0.0338)	0.0733(0.1698)	-	-	-	0.0169(0.0090)	-	-
ν_{38}(0.1381)	-	-	-	-	-	0.0249(0.0163)	0.0394(0.0407)	-	-	-	0.0072(0.0014)	-	-
ν_{39}(0.1397)	0.0129(0.0043)	-	0.0441(0.0498)	-	-	-	-	-	-	0.0240(0.0148)	-	-	0.0191(0.0093)
ν_{40}(0.1445)	-	-	-	-	-	-	-	-	-	-	-	-	-
ν_{42}(0.1486)	0.0087(0.0017)	-	0.0381(0.0017)	-	-	-	-	-	-	-	-	-	-
ν_{43}(0.1493)	-	-	-	-	-	-	-	0.0432(0.0419)	-	-	-	0.0271(0.0165)	-
ν_{44}(0.1528)	-	0.0198(0.0084)	-	-	-	-	-	0.0037(0.0003)	-	-	-	0.0124(0.0033)	-
ν_{46}(0.1567)	0.0068(0.0009)	-	0.0355(0.0257)	-	-	-	-	-	-	-	-	-	-
ν_{47}(0.1573)	-	-	-	-	0.0276(0.0154)	0.0359(0.0260)	0.0790(0.1261)	-	-	-	0.0189(0.0072)	-	-
ν_{48}(0.1665)		–	-	-	-	-	-	-	-	-	-	0.0397(0.0284)	-
ν_{50}(0.1736)	0.0254(0.0107)	-	0.0954(0.1510)	-	-	-	-	-	-	0.0975(0.1577)	-	-	0.0563(0.0526)
ν_{52}(0.1778)	0.0073(0.0008)	-	0.0184(0.0054)	-	-	-	-	-	-	-	-	-	-
ν_{53}(0.1807)	-	0.0652(0.0651)	-	0.0359(0.0197)	-	-	-	0.0276(0.0117)	-	-	-	-	-
ν_{54}(0.1810)	-	-	-	-	-	0.0222(0.0075)	0.1531(0.3577)	-	-	-	0.0502(0.0385)	-	-
ν_{55}(0.1839)	-	-	-	-	-	0.0533(0.0420)	0.1874(0.5192)	-	-	-	0.0603(0.0538)	-	-
ν_{56}(0.1879)	-	0.0863(0.1055)	-	0.0782(0.0866)	-	-	-	0.0337(0.0161)	-	-	-	-	-
ν_{57}(0.1904)	0.0024(0.0001)	-	-	-	-	-	-	-	-	-	-	-	-
ν_{59}(0.2016)	0.0387(0.0184)	-	0.1404(0.2425)	-	-	-	-	-	-	0.1151(0.1630)	-	-	0.0594(0.0434)
ν_{60}(0.2028)	-	-	-	-	0.0636(0.0492)	0.0330(0.0132)	0.1463(0.2602)	-	-	-	0.0486(0.0287)	-	-
ν_{61}(0.2041)	-	0.0228(0.0062)	-	0.0596(0.0426)	-	-	-	0.0693(0.0576)	-	-	-	0.0593(0.0422)	-
ν_{63}(0.3913)	-	-	-	-	0.0048(0.0001)	-	0.0237(0.0018)	-	-	-	0.0054(0.0001)	-	-
ν_{64}(0.3913)	0.0018(0.0001)	-	0.0050(0.0001)	-	-	-	-	-	-	0.0108(0.0001)	-	-	-
ν_{66}(0.3918)	-	-	-	-	0.0042(0.0001)	0.0071(0.0002)	-	-	-	-	-	-	-
ν_{67}(0.3927)	-	0.0178(0.0010)	-	-	-	-	-	0.0009(0.0001)	-	-	-	0.0045(0.0001)	-
ν_{68}(0.3928)	0.0038(0.0001)	-	0.0096(0.0001)	-	-	-	-	-	-	-	-	-	0.0087(0.0001)
ν_{70}(0.3937)	-	-	-	0.0179(0.0010)	-	-	-	-	-	-	-	0.0014(0.0001)	-
ν_{71}(0.3948)	-	-	-	-	0.0038(0.0001)	0.0085(0.0002)	0.0048(0.0001)	-	-	-	0.0004(0.0001)	-	

Table S8: Linear intrastate coupling parameters (κ) for triplet electronic states of **P** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

AG mode (Freq, eV)	κ^{T_1}	κ^{T_2}	κ^{T_3}	κ^{T_4}	κ^{T_5}	κ^{T_6}
ν_8(0.0511)	-0.0557(0.5946)	-0.0168(0.0537)	-0.0009(0.0002)	-0.0416(0.3321)	-0.0352(0.2375)	0.0276(0.1454)
ν_{17}(0.0738)	-0.0058(0.0031)	-0.0308(0.0868)	-0.0291(0.0778)	-0.0411(0.1553)	-0.0749(0.5149)	-0.0531(0.2589)
ν_{25}(0.1010)	-0.0128(0.0080)	0.0050(0.0012)	-0.0004(0.0001)	-0.0211(0.0218)	-0.0022(0.0002)	0.0230(0.0259)
ν_{37}(0.1353)	-0.0199(0.0108)	-0.0531(0.0769)	0.0115(0.0036)	-0.0434(0.0515)	-0.0889(0.2157)	-0.0363(0.0359)
ν_{41}(0.1448)	-0.0530(0.0669)	0.0139(0.0046)	-0.0990(0.2336)	0.0088(0.0018)	-0.0312(0.0233)	0.0607(0.0878)
ν_{45}(0.1565)	0.1570(0.5032)	0.0897(0.1532)	-0.0176(0.0063)	0.0909(0.1688)	0.0085(0.0015)	0.0685(0.0957)
ν_{49}(0.1676)	-0.0136(0.0033)	-0.0181(0.0058)	-0.0562(0.0563)	-0.0267(0.0127)	-0.0403(0.0289)	0.0892(0.1415)
ν_{51}(0.1770)	-0.1141(0.2079)	-0.1086(0.1883)	-0.0489(0.0382)	-0.1184(0.2237)	-0.0924(0.1364)	0.0232(0.0086)
ν_{58}(0.1979)	-0.0219(0.0061)	0.0539(0.0371)	0.0999(0.1273)	0.0435(0.0241)	-0.0984(0.1236)	0.1457(0.2710)
ν_{62}(0.2072)	0.2454(0.7012)	-0.0091(0.0010)	0.2505(0.7308)	0.0023(0.0001)	0.1099(0.1407)	-0.2028(0.4790)
ν_{65}(0.3917)	-0.0099(0.0003)	0.0039(0.0001)	0.0014(0.0001)	-0.0056(0.0001)	-0.0114(0.0004)	0.0089(0.0003)
ν_{69}(0.3937)	-0.0084(0.0002)	0.0002(0.0001)	-0.0319(0.0033)	-0.0044(0.0001)	-0.0026(0.0001)	0.0005(0.0001)
ν_{72}(0.3949)	0.0119(0.0005)	0.0173(0.0010)	0.0077(0.0002)	0.0147(0.0007)	0.0136(0.0006)	0.0205(0.0013)

Table S9: Linear interstate coupling parameters (λ) for triplet electronic states of **P** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

Vibrational mode (Freq, eV)	$\lambda_{T_1-T_2}$	$\lambda_{T_1}-T_3$	$\lambda_{T_1}-T_4$	$\lambda_{T_1}-T_5$	$\lambda_{T_2}-T_3$	$\lambda_{T_2}-T_5$	$\lambda_{T_2}-T_6$	$\lambda_{T_3}-T_4$	$\lambda_{T_3}-T_5$	$\lambda_{T_3}-T_6$	$\lambda_{T_4}-T_5$	$\lambda_{T_4}-T_6$	$\lambda_{T_5}-T_6$
ν_6(0.0446)	-	0.0272(0.1860)	-	-	-	-	-	-	-	0.0120(0.0362)	0.0083 (0.0173)	-	-
ν_9(0.0574)	0.0308(0.1440)	-	0.0318 (0.1535)	-	-	-	0.0210(0.0669)	-	0.0340 (0.1754)	-	-	0.0185 (0.0519)	-
ν_{11}(0.0629)	-	-	-	-	0.0099 (0.0124)	-	-	-	-	-	-	-	0.0139 (0.0244)
ν_{12}(0.0631)	0.0400(0.2009)	-	0.0405 (0.2060)	-	-	-	0.0222(0.0619)	-	0.0087 (0.0095)	-	-	0.0190 (0.0453)	-
ν_{15}(0.0687)	-	0.0234(0.0580)	-	-	-	0.0069 (0.0050)	-	-	-	-	0.0085 (0.0077)	-	-
ν_{19}(0.0873)	-	-	-	-	0.0260 (0.0443)	-	-	-	-	-	-	-	0.0131 (0.0113)
ν_{21}(0.0929)	-	-	-	-	-	-	0.0118(0.0081)	-	-	-	-	0.0102 (0.0060)	-
ν_{26}(0.1035)	-	-	-	-	-	-	-	0.0133(0.0083)	-	-	-	-	0.0197 (0.0181)
ν_{33}(0.1216)	-	-	-	-	-	0.0298 (0.0300)	-	-	-	0.0177(0.0106)	0.0176 (0.0105)	-	-
ν_{36}(0.1258)	-	-	-	-	0.0348 (0.0383)	-	-	-	-	-	-	-	0.0219 (0.0152)
ν_{38}(0.1381)	-	-	-	-	0.0068 (0.0012)	-	-	0.0065(0.0011)	-	-	-	-	0.0275 (0.0198)
ν_{39}(0.1397)	0.0505(0.0653)	-	0.0301 (0.0232)	-	-	-	0.0315(0.0254)	-	0.0540 (0.0747)	-	-	0.0326 (0.0272)	-
ν_{40}(0.1445)	-	-	-	-	-	-	-	-	-	0.0298(0.0213)	-	-	-
ν_{42}(0.1486)	0.0435(0.0428)	-	0.0509 (0.0587)	-	-	-	0.0316(0.0226)	-	-	-	-	0.0239 (0.0129)	-
ν_{43}(0.1493)	-	-	-	-	-	0.0481 (0.0519)	-	-	-	0.0313(0.0220)	0.0273 (0.0167)	-	-
ν_{44}(0.1528)	-	-	-	-	-	0.0458 (0.0449)	-	-	-	0.0344(0.0253)	0.0196 (0.0082)	-	-
ν_{46}(0.1567)	-	-	0.0181 (0.0067)	-	-	-	0.0150(0.0046)	-	0.0186 (0.0070)	-	-	-	-
ν_{47}(0.1573)	-	-	-	-	0.0475 (0.0456)	-	-	-	-	-	-	-	0.0077 (0.0012)
ν_{48}(0.1665)	-	-	-	-	-	-	-	-	-	0.0345(0.0215)	-	-	-
ν_{50}(0.1736)	0.0850(0.1199)	-	0.0992 (0.1633)	-	-	-	0.0503(0.0420)	-	0.0844 (0.1182)	-	-	0.0364 (0.0220)	-
ν_{52}(0.1778)	0.0228(0.0082)	-	0.0121 (0.0023)	-	-	-	0.0152(0.0037)	-	0.0077 (0.0009)	-	-	0.0165 (0.0043)	-
ν_{53}(0.1807)	-	0.0873(0.1167)	-	-	-	0.0319 (0.0156)	-	-	-	-	0.0292 (0.0131)	-	-
ν_{54}(0.1810)	-	-	-	-	0.0227 (0.0079)	-	-	0.0034(0.0002)	-	-	-	-	0.0187 (0.0053)
ν_{55}(0.1839)	-	-	-	-	0.0674(0.0672)	-	-	-)	-	-	-	-	0.0344 (0.0175)
ν_{56}(0.1879)	-	0.1481(0.3106)	-	-	-	0.0678 (0.0651)	-	-	-	-	0.0387 (0.0212)	-	-
ν_{57}(0.1904)	0.0307(0.0130)	-	0.0463 (0.0296)	-	-	-	0.0226(0.0070)	-	0.0227 (0.0071)	-	-	0.0101 (0.0014)	-
ν_{59}(0.2016)	0.1371(0.2312)	-	0.1465 (0.2640)	-	-	-	0.0914(0.1028)	-	0.1416 (0.2467)	-	-	0.0751 (0.0694)	-
ν_{60}(0.2028)	-	-	-	-	0.0337 (0.0138)	-	-	-	-	-	-	-	0.0635 (0.0490)
ν_{61}(0.2041)	-	0.0692(0.0575)	-	-	-	0.0771 (0.0713)	-	-	-	0.0627(0.0472)	-	-	-
ν_{63}(0.3913)	-	-	-	-	-	-	-	0.0033(0.0001)	-	-	-	-	0.0018 (0.0001)
ν_{64}(0.3913)	0.0130(0.0006)	-	0.0099 (0.0003)	-	-	-	0.0043(0.0001)	-	0.0128 (0.0005)	-	-	0.0061 (0.0001)	-
ν_{66}(0.3918)	-	-	-	-	-	-	-	0.0020(0.0001)	-	-	-	-	0.0005 (0.0001)
ν_{67}(0.3927)	-	0.0136(0.0006)	-	-	-	0.0059 (0.0001)	-	-	-	-	0.0047 (0.0001)	-	-
ν_{68}(0.3928)	0.0135(0.0006)	-	-	-	-	-	0.0073(0.0002)	-	-	-	-	0.0119 (0.0005)	-
ν_{70}(0.3937)	-	-	-	-	-	-	-	-	-	0.0118(0.0004)	0.0042 (0.0001)	-	-
ν_{71}(0.3948)	-	-	-	-	0.0040 (0.0001)	-	-	-	-	-	-	-	0.0056 (0.0001)

Table S10: Linear intrastate coupling parameters (κ) for singlet electronic states of **AP2** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

A mode (Freq, eV)	κ^{S_1}	κ^{S_2}	κ^{S_3}	κ^{S_4}	κ^{S_5}	κ^{S_6}
ν_1(0.0060)	0.0141(2.7613)	0.0243(8.2013)	0.0361(18.0946)	0.0233(7.5452)	0.0140(2.7296)	0.0069(0.6594)
ν_3(0.0077)	0.0024(0.0486)	0.0124(1.2967)	0.0254(5.4433)	0.0137(1.5772)	0.0147(1.8321)	0.0105(0.9226)
ν_6(0.0181)	-0.0029(0.0128)	-0.0003(0.0001)	0.0043(0.0289)	0.0075(0.0862)	0.0046(0.0324)	0.0001(0.0001)
ν_7(0.0208)	0.0026(0.0078)	0.0148(0.2531)	0.0194(0.4347)	0.0093(0.0993)	0.0035(0.0145)	0.0022(0.0056)
ν_{10}(0.0233)	0.0038(0.0133)	-0.0008(0.0006)	-0.0019(0.0034)	-0.0038(0.0132)	-0.0126(0.1459)	-0.0152(0.2133)
ν_{12}(0.0331)	0.0059(0.0159)	-0.0009(0.0004)	-0.0127(0.0738)	-0.0004(0.0001)	0.0020(0.0018)	0.0078(0.0278)
ν_{15}(0.0383)	0.0105(0.0376)	-0.0036(0.0044)	-0.0002(0.0001)	0.0078(0.0210)	0.0200(0.1364)	0.0181(0.1112)
ν_{17}(0.0453)	-0.0144(0.0505)	-0.0072(0.0126)	-0.0136(0.0452)	-0.0055(0.0073)	-0.0298(0.2159)	-0.0234(0.1334)
ν_{18}(0.0526)	-0.0232(0.0973)	-0.0113(0.0231)	-0.0024(0.0011)	0.0020(0.0007)	-0.0317(0.1813)	-0.0283(0.1448)
ν_{20}(0.0601)	0.0068(0.0064)	0.0118(0.0193)	0.0174(0.0421)	-0.0104(0.0148)	0.0134(0.0247)	0.0130(0.0235)
ν_{24}(0.0661)	0.0085(0.0083)	-0.0031(0.0011)	-0.0129(0.0192)	-0.0201(0.0464)	-0.0029(0.0010)	0.0024(0.0006)
ν_{26}(0.0689)	0.0061(0.0039)	0.0035(0.0013)	0.0063(0.0042)	-0.0161(0.0273)	-0.0026(0.0007)	-0.0061(0.0039)
ν_{28}(0.0733)	-0.0040(0.0015)	0.0164(0.0250)	0.0318(0.0942)	-0.0053(0.0026)	-0.0178(0.0295)	-0.0260(0.0628)
ν_{30}(0.0802)	-0.0005(0.0001)	0.0106(0.0087)	0.0025(0.0005)	-0.0030(0.0007)	-0.0089(0.0061)	-0.0125(0.0121)
ν_{32}(0.0822)	0.0078(0.0045)	0.0306(0.0693)	0.0417(0.1285)	0.0292(0.0629)	0.0232(0.0398)	0.0204(0.0309)
ν_{34}(0.0877)	0.0113(0.0083)	0.0182(0.0215)	0.0152(0.0149)	0.0076(0.0037)	0.0183(0.0219)	-0.0123(0.0099)
ν_{35}(0.0892)	0.0005(0.0001)	0.0076(0.0036)	0.0097(0.0060)	-0.0019(0.0002)	0.0070(0.0031)	-0.0014(0.0001)
ν_{38}(0.1026)	0.0015(0.0001)	-0.0036(0.0006)	0.0072(0.0025)	0.0078(0.0029)	0.0036(0.0006)	0.0072(0.0024)
ν_{40}(0.1031)	0.0136(0.0087)	-0.0066(0.0020)	-0.0004(0.0001)	0.0027(0.0003)	0.0199(0.0185)	-0.0121(0.0068)
ν_{43}(0.1074)	0.0008(0.0001)	0.0114(0.0056)	0.0138(0.0082)	0.0160(0.0112)	0.0503(0.1096)	0.0330(0.0471)
ν_{44}(0.1138)	-0.0063(0.0015)	0.0002(0.0001)	-0.0001(0.0001)	-0.0025(0.0002)	-0.0023(0.0002)	-0.0003(0.0001)
ν_{46}(0.1210)	0.0064(0.0014)	0.0058(0.0011)	0.0144(0.0071)	0.0078(0.0021)	0.0187(0.0120)	0.0062(0.0013)
ν_{48}(0.1224)	0.0013(0.0001)	0.0063(0.0013)	0.0050(0.0008)	0.0008(0.0001)	0.0108(0.0039)	0.0114(0.0043)
ν_{52}(0.1282)	-0.0158(0.0076)	-0.0167(0.0085)	-0.0089(0.0024)	0.0005(0.0001)	-0.0074(0.0017)	-0.0059(0.0010)
ν_{54}(0.1314)	0.0017(0.0001)	-0.0125(0.0045)	-0.0173(0.0086)	-0.0066(0.0013)	0.0118(0.0040)	0.0224(0.0145)
ν_{55}(0.1369)	-0.0173(0.0080)	0.0024(0.0002)	0.0162(0.0070)	-0.0200(0.0107)	-0.0026(0.0002)	-0.0065(0.0011)
ν_{57}(0.1446)	-0.0354(0.0300)	0.0125(0.0037)	0.0279(0.0186)	0.0059(0.0008)	-0.0092(0.0020)	-0.0152(0.0055)
ν_{59}(0.1480)	0.0050(0.0006)	0.0145(0.0048)	0.0204(0.0095)	-0.0004(0.0001)	-0.0280(0.0179)	-0.0242(0.0133)
ν_{64}(0.1574)	0.0963(0.1872)	0.0951(0.1825)	0.1076(0.2336)	0.0905(0.1654)	0.0690(0.0962)	0.0678(0.0928)
ν_{65}(0.1584)	0.0201(0.0081)	0.0497(0.0492)	0.0669(0.0893)	0.0302(0.0181)	0.0317(0.0201)	0.0390(0.0302)
ν_{67}(0.1694)	-0.0048(0.0004)	-0.0066(0.0008)	-0.0355(0.0219)	-0.0005(0.0001)	0.0288(0.0144)	0.0298(0.0155)
ν_{68}(0.1718)	-0.0298(0.0150)	-0.0416(0.0293)	-0.0451(0.0345)	-0.0352(0.0210)	0.0154(0.0040)	0.0033(0.0002)
ν_{70}(0.1727)	-0.0559(0.0524)	-0.0112(0.0021)	0.0164(0.0045)	-0.0397(0.0265)	0.0072(0.0009)	-0.0129(0.0028)
ν_{73}(0.1790)	0.0316(0.0156)	0.0304(0.0144)	0.0543(0.0459)	0.0290(0.0132)	0.0397(0.0246)	0.0015(0.0001)
ν_{76}(0.1829)	0.0011(0.0001)	0.0081(0.0010)	0.0159(0.0038)	0.0093(0.0013)	0.0099(0.0015)	-0.0056(0.0005)
ν_{78}(0.1840)	-0.0098(0.0014)	-0.0205(0.0062)	-0.0309(0.0141)	-0.0122(0.0022)	-0.0117(0.0020)	0.0122(0.0022)
ν_{79}(0.1847)	-0.0098(0.0014)	0.0112(0.0018)	0.0096(0.0013)	0.0025(0.0001)	-0.0251(0.0092)	0.0099(0.0014)
ν_{82}(0.1926)	0.0401(0.0217)	0.0256(0.0088)	0.0411(0.0227)	-0.0199(0.0053)	0.0016(0.0001)	-0.0108(0.0016)
ν_{84}(0.2012)	0.0328(0.0133)	0.0319(0.0126)	0.0348(0.0150)	0.0291(0.0104)	0.0560(0.0387)	0.0231(0.0066)
ν_{86}(0.2065)	-0.1260(0.1862)	-0.0558(0.0365)	-0.0779(0.0712)	-0.0079(0.0007)	-0.1370(0.2202)	-0.1481(0.2572)
ν_{88}(0.2177)	-0.0525(0.0291)	-0.1020(0.1098)	-0.1503(0.2384)	-0.0500(0.0264)	-0.0507(0.0272)	-0.0496(0.0260)
ν_{90}(0.3765)	0.0077(0.0002)	-0.0035(0.0001)	-0.0025(0.0001)	0.0023(0.0001)	0.0092(0.0003)	0.0085(0.0003)
ν_{91}(0.3847)	0.0003(0.0001)	-0.0005(0.0001)	-0.0009(0.0001)	0.0001(0.0001)	-0.0018(0.0001)	-0.0027(0.0001)
ν_{94}(0.3889)	-0.0006(0.0001)	0.0086(0.0002)	0.0096(0.0003)	0.0012(0.0001)	-0.0015(0.0001)	0.0010(0.0001)
ν_{95}(0.3922)	0.0006(0.0001)	0.0026(0.0001)	0.0019(0.0001)	0.0020(0.0001)	0.0018(0.0001)	0.0034(0.0001)
ν_{97}(0.3929)	-0.0072(0.0002)	-0.0042(0.0001)	-0.0038(0.0001)	-0.0055(0.0001)	-0.0121(0.0005)	-0.0067(0.0001)
ν_{99}(0.3954)	0.0041(0.0001)	0.0009(0.0001)	-0.0004(0.0001)	0.0068(0.0001)	0.0057(0.0001)	0.0045(0.0001)
ν_{100}(0.3983)	-0.0021(0.0001)	-0.0031(0.0001)	-0.0016(0.0001)	-0.0049(0.0001)	-0.0032(0.0001)	-0.0025(0.0001)
ν_{102}(0.3999)	-0.0011(0.0001)	0.0011(0.0001)	0.0023(0.0001)	-0.0015(0.0001)	-0.0039(0.0001)	-0.0064(0.0001)

Table S11: Linear interstate coupling parameters (λ) for singlet electronic states of **AP2** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

B mode (Freq, eV)	$\lambda_{S_1-S_2}$	$\lambda_{S_1-S_4}$	$\lambda_{S_1-S_5}$	$\lambda_{S_1-S_6}$	$\lambda_{S_2-S_3}$	$\lambda_{S_3-S_4}$	$\lambda_{S_3-S_5}$	$\lambda_{S_3-S_6}$
ν_2(0.0062)	0.0018(0.0421)	0.0383(19.0803)	0.0043(0.2405)	-	-	0.0096(1.1988)	0.0505(33.1718)	0.0516(34.6327)
ν_4(0.0080)	0.0083(0.5382)	0.0326(8.3028)	0.0218(3.7128)	0.0183(2.6163)	-	0.0063(0.3101)	0.0359(10.0688)	0.0395(12.1895)
ν_5(0.0156)	0.0067(0.0922)	0.0451(4.1790)	-	-	-	0.0119(0.2909)	0.0556(6.3514)	0.0644(8.5210)
ν_8(0.0214)	0.0084(0.0770)	0.0365(1.4545)	-	-	-	0.0077(0.0647)	0.0317(1.0971)	0.0338(1.2473)
ν_9(0.0217)	0.0026(0.0072)	0.0547(3.1771)	-	-	-	0.0153(0.2486)	0.0658(4.5973)	0.0753(6.0206)
ν_{11}(0.0285)	0.0078(0.0375)	0.0364(0.8156)	0.0255(0.4003)	0.0131(0.1056)	-	0.0079(0.0384)	0.0457(1.2856)	0.0487(1.4600)
ν_{13}(0.0336)	0.0120(0.0638)	0.0558(1.3790)	-	0.0047(0.0098)	-	0.0153(0.1037)	0.0624(1.7245)	0.0732(2.3731)
ν_{14}(0.0372)	0.0062(0.0139)	0.0362(0.4735)	0.0256(0.2368)	0.0211(0.1609)	-	0.0070(0.0177)	0.0386(0.5383)	0.0418(0.6313)
ν_{16}(0.0429)	0.0199(0.1076)	0.0266(0.1922)	0.0409(0.4545)	0.0404(0.4434)	-	0.0012(0.0004)	0.0083(0.0187)	-
ν_{19}(0.0538)	0.0144(0.0358)	0.0291(0.1463)	0.0285(0.1403)	0.0192(0.1403)	-	0.0038(0.0025)	0.0195(0.0657)	0.0129(0..0287)
ν_{21}(0.0609)	0.0109(0.0160)	0.0356(0.1709)	-	-	-	0.0076(0.0078)	0.0386(0.2009)	0.0407(0.2233)
ν_{22}(0.0631)	0.0092(0.0106)	0.0159(0.0317)	0.0217(0.0591)	-	-	0.0003(0.0001)	-	-
ν_{23}(0.0635)	0.0110(0.0150)	0.0188(0.0438)	-	-	0.0105(0.0137)	-	-	-
ν_{25}(0.0662)	0.0157(0.0281)	0.0623(0.4428)	0.0305(0.1061)	0.0255(.0742)	-	0.0167(0.0318)	0.0667(0.5076)	0.0748(0.6383)
ν_{27}(0.0699)	0.0069(0.0049)	0.0732(0.5483)	0.0242(0.0599)	0.0238(0.0580)	-	0.0253(0.0655)	0.0920(0.8661)	0.1057(1.1433)
ν_{29}(0.0777)	0.0079(0.0052)	0.0560(0.2597)	0.0269(0.0599)	0.0152(0.0191)	-	0.0153(0.0194)	0.0671(0.3729)	0.0745(0.4597)
ν_{31}(0.0810)	-	0.0015(0.0002)	-	-	0.0136(0.0141)	-	-	-
ν_{33}(0.0877)	0.0033(0.0007)	0.0286(0.0532)	0.0169(0.0186)	0.0047(0.0014)	-	0.0056(0.0020)	0.0346(0.0778)	0.0377(0.0924)
ν_{36}(0.0910)	-	0.0230(0.0319)	-	-	-	0.0051(0.0016)	0.0314(0.0595)	0.0240(0.0348)
ν_{37}(0.0956)	0.0094(0.0048)	0.0237(0.0307)	0.0231(0.0292)	0.0142(0.0110)	-	0.0031(0.0005)	0.0177(0.0171)	0.0118(0.0076)
ν_{39}(0.1030)	0.0119(0.0067)	0.0191(0.0172)	-	-	-	0.0009(0.0001)	-	-
ν_{41}(0.1045)	-	0.0260(0.0310)	0.0255(0.0298)	0.0297(0.0404)	0.0094(0.0040)	0.0034(0.0005)	0.0200(0.0183)	0.0246(0.0277)
ν_{42}(0.1062)	0.0090(0.0036)	0.0100(0.0044)	0.0181(0.0145)	0.0095(0.0040)	-	-	-	-
ν_{45}(0.1180)	0.0135(0.0065)	0.0454(0.0740)	0.0222(0.0177)	0.0181(0.0118)	-	0.0109(0.0043)	0.0528(0.1001)	0.0595(0.1271)
ν_{47}(0.1216)	0.0081(0.0022)	0.0113(0.0043)	-	-	-	0.0001(0.0001)	-	-
ν_{49}(0.1231)	0.0060(0.0012)	0.0026(0.0002)	-	-	-	0.0008(0.0001)	0.0076(0.0019)	-
ν_{50}(0.1239)	0.0102(0.0034)	0.0208(0.0141)	0.0174(0.0099)	0.0126(0.0052)	-	0.0032(0.0003)	0.0216(0.0152)	0.0222(0.0161)
ν_{51}(0.1263)	0.0097(0.0029)	0.0359(0.0404)	0.0290(0.0264)	0.0230(0.0166)	-	0.0069(0.0015)	0.0396(0.0492)	0.0419(0.0550)
ν_{53}(0.1289)	0.0020(0.0001)	0.0165(0.0082)	-	-	-	0.0036(0.0004)	0.0275(0.0228)	0.0276(0.0229)
ν_{56}(0.1405)	-	0.0284(0.0204)	-	0.0123(0.0038)	-	0.0051(0.0007)	0.0278(0.0196)	0.0331(0.0278)
ν_{58}(0.1470)	-	0.0345(0.0275)	0.0183(0.0077)	-	-	0.0080(0.0015)	0.0463(0.0496)	0.0493(0.0562)
ν_{60}(0.1488)	-	0.0511(0.0590)	0.0331(0.0247)	0.0324(0.0237)	-	0.0130(0.0038)	0.0629(0.0893)	0.0713(0.1148)
ν_{61}(0.1502)	-	0.0634(0.0890)	0.0086(0.0016)	-	-	0.0204(0.0092)	0.0811(0.1458)	0.0923(0.1888)
ν_{62}(0.1541)	-	0.0869(0.1590)	0.0240(0.0121)	0.0249(0.0131)	-	0.0300(0.0189)	0.0933(0.1833)	0.1074(0.2429)
ν_{63}(0.1556)	-	0.0672(0.0933)	0.0129(0.0034)	0.0175(0.0063)	-	0.0203(0.0085)	0.0756(0.1180)	0.0877(0.1588)
ν_{66}(0.1659)	-	0.0348(0.0220)	-	-	-	0.0082(0.0012)	0.0394(0.0282)	0.0429(.0334)
ν_{69}(0.1719)	-	0.0665(0.0748)	-	-	-	0.0210(0.0075)	0.0794(0.1067)	0.0907(0.1392)
ν_{71}(0.1730)	0.0229(0.0088)	0.0663(0.0734)	-	0.0392(0.0257)	-	0.0149(0.0037)	0.0484(0.0391)	0.0571(0.0545)
ν_{72}(0.1751)	0.0105(0.0018)	0.0370(0.0224)	0.0341(0.0189)	0.0456(0.0339)	-	0.0063(0.0006)	0.0356(0.0207)	0.0466(0.0354)
ν_{74}(0.1793)	0.0026(0.0001)	0.0174(0.0047)	0.0216(0.0072)	0.0176(0.0048)	-	0.0027(0.0001)	0.0228(0.0081)	0.0229(0.0081)
ν_{75}(0.1828)	-	0.0334(0.0167)	0.0158(0.0037)	0.0136(0.0028)	-	0.0076(0.0009)	0.0444(0.0295)	0.0506(0.0384)
ν_{77}(0.1839)	-	0.0401(0.0237)	0.0152(0.0034)	0.0142(0.0030)	-	0.0097(0.0014)	0.0508(0.0382)	0.0583(0.0503)
ν_{80}(0.1880)	0.0055(0.0004)	0.0433(0.0265)	0.0592(0.0496)	0.0577(0.0471)	-	0.0084(0.0010)	0.0579(0.0474)	0.0620(0.0544)
ν_{81}(0.1909)	-	0.0598(0.0490)	0.0324(0.0144)	0.0317(0.0138)	-	0.0159(0.0035)	0.0668(0.0612)	0.0759(0.0789)
ν_{83}(0.2003)	0.0304(0.0115)	0.0911(0.1033)	0.0719(0.0645)	0.0768(0.0736)	-	0.0234(0.0068)	0.0729(0.0663)	0.0828(0.0854)
ν_{85}(0.2040)	0.0045(0.0002)	0.0486(0.0284)	0.0320(0.0123)	0.0511(0.0314)	-	0.0098(0.0012)	0.0429(0.0221)	0.0587(0.0415)
ν_{87}(0.2172)	-	0.1243(0.1637)	0.0827(0.0726)	0.0733(0.0570)	0.0174(0.0032)	0.0432(0.0198)	0.1098(0.1277)	0.1169(0.1449)
ν_{89}(0.3765)	0.0036(0.0001)	0.0157(0.0009)	-	-	-	0.0023(0.0001)	0.0136(0.0006)	0.0080(0.0002)
ν_{92}(0.3847)	0.0038(0.0001)	0.0105(0.0004)	-	-	-	0.0011(0.0001)	-	-
ν_{93}(0.3889)	0.0060(0.0001)	0.0205(0.0014)	0.0097(0.0003)	-	-	0.0030(0.0001)	0.0154(0.0008)	0.0167(0.0009)
ν_{96}(0.3927)	-	0.0026(0.0001)	0.0153(0.0008)	0.0172(0.0010)	-	0.0006(0.0001)	0.0113(0.0004)	0.0133(0.0006)
ν_{98}(0.3933)	-	0.0040(0.0001)	0.0134(0.0006)	0.0071(0.0002)	-	0.0009(0.0001)	0.0115(0.0004)	0.0108(0.0004)
ν_{101}(0.3999)	-	0.0053(0.0001)	0.0187(0.0011)	0.0148(0.0007)	-	0.0008(0.0001)	0.0172(0.0009)	0.0138(0.0006)

Table S12: Linear intrastate coupling parameters (κ) for triplet electronic states of **AP2** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

A mode (Freq, eV)	κ^{T_1}	κ^{T_2}	κ^{T_3}	κ^{T_4}	κ^{T_5}	κ^{T_6}
ν_1(0.0060)	0.0135(2.5313)	0.0194(5.2272)	0.0269(10.0501)	0.0303(12.7513)	0.0072(0.7200)	0.0038(0.2006)
ν_3(0.0077)	0.0061(0.3138)	0.0143(1.7245)	0.0176(2.6122)	0.0182(2.7934)	0.0077(0.5000)	0.0012(0.0121)
ν_6(0.0181)	-0.0042(0.0269)	-0.0050(0.0382)	0.0049(0.0366)	0.0058(0.0513)	-0.0007(0.0007)	0.0111(0.1880)
ν_7(0.0208)	0.0010(0.0012)	0.0098(0.1110)	0.0117(0.1582)	0.0114(0.1502)	0.0006(0.0004)	0.0006(0.0004)
ν_{10}(0.0233)	0.0043(0.0170)	-0.0033(0.0100)	-0.0060(0.0332)	-0.0008(0.0006)	-0.0059(0.0321)	-0.0083(0.0634)
ν_{12}(0.0331)	-0.0008(0.0003)	0.0100(0.0456)	0.0023(0.0024)	-0.0039(0.0069)	0.0009(0.0004)	0.0033(0.0050)
ν_{15}(0.0383)	0.0220(0.1650)	-0.0113(0.0435)	-0.0068(0.0158)	0.0075(0.0192)	0.0209(0.1489)	0.0138(0.0649)
ν_{17}(0.0453)	-0.0240(0.1403)	0.0033(0.0027)	-0.0024(0.0014)	-0.0051(0.0063)	-0.0249(0.1511)	-0.0118(0.0339)
ν_{18}(0.0526)	-0.0339(0.2077)	-0.0089(0.0143)	-0.0059(0.0063)	0.0121(0.0265)	-0.0294(0.1562)	-0.0248(0.1111)
ν_{20}(0.0601)	0.0168(0.0391)	0.0076(0.0080)	0.0176(0.0429)	-0.0171(0.0405)	0.0156(0.0337)	0.0124(0.0213)
ν_{24}(0.0661)	0.0094(0.0101)	0.0027(0.0008)	-0.0032(0.0012)	-0.0328(0.1231)	-0.0027(0.0008)	0.0111(0.0141)
ν_{26}(0.0689)	0.0054(0.0031)	0.0074(0.0058)	-0.0153(0.0247)	0.0096(0.0097)	0.0032(0.0011)	-0.0084(0.0074)
ν_{28}(0.0733)	-0.0007(0.0001)	0.0007(0.0001)	0.0130(0.0157)	-0.0025(0.0006)	-0.0133(0.0165)	-0.0134(0.0167)
ν_{30}(0.0802)	-0.0026(0.0005)	0.0155(0.0187)	0.0032(0.0008)	-0.0117(0.0106)	0.0024(0.0004)	0.0136(0.0144)
ν_{32}(0.0822)	-0.0006(0.0001)	0.0265(0.0520)	0.0419(0.1299)	0.0252(0.0470)	0.0229(0.0388)	0.0385(0.1097)
ν_{34}(0.0877)	0.0100(0.0065)	0.0174(0.0197)	0.0138(0.0124)	0.0042(0.0011)	-0.0006(0.0001)	0.0122(0.0097)
ν_{35}(0.0892)	-0.0005(0.0001)	0.0035(0.0008)	0.0029(0.0005)	-0.0030(0.0006)	0.0097(0.0059)	0.0050(0.0016)
ν_{38}(0.1026)	0.0081(0.0031)	-0.0050(0.0012)	0.0009(0.0001)	0.0094(0.0042)	0.0018(0.0002)	0.0023(0.0003)
ν_{40}(0.1031)	0.0070(0.0023)	-0.0057(0.0015)	-0.0008(0.0001)	-0.0051(0.0012)	0.0116(0.0063)	0.0023(0.0002)
ν_{43}(0.1074)	0.0013(0.0001)	0.0219(0.0208)	0.0137(0.0081)	0.0285(0.0352)	0.0191(0.0158)	-0.0106(0.0049)
ν_{44}(0.1138)	-0.0040(0.0006)	0.0002(0.0001)	0.0006(0.0001)	-0.0019(0.0001)	0.0004(0.0001)	-0.0013(0.0001)
ν_{46}(0.1210)	0.0072(0.0018)	-0.0033(0.0004)	-0.0008(0.0001)	0.0161(0.0089)	0.0066(0.0015)	-0.0088(0.0026)
ν_{48}(0.1224)	0.0027(0.0002)	0.0023(0.0002)	0.0020(0.0001)	0.0039(0.0005)	0.0126(0.0053)	-0.0013(0.0001)
ν_{52}(0.1282)	-0.0130(0.0051)	-0.0223(0.0151)	-0.0158(0.0076)	-0.0010(0.0001)	-0.0055(0.0009)	0.0043(0.0006)
ν_{54}(0.1314)	-0.0055(0.0009)	0.0002(0.0001)	-0.0144(0.0060)	-0.0038(0.0004)	0.0136(0.0054)	-0.0077(0.0017)
ν_{55}(0.1369)	-0.0217(0.0126)	-0.0079(0.0017)	0.0119(0.0038)	-0.0153(0.0062)	0.0029(0.0002)	-0.0245(0.0160)
ν_{57}(0.1446)	-0.0557(0.0742)	0.0063(0.0009)	0.0225(0.0121)	0.0170(0.0069)	-0.0224(0.0120)	-0.0166(0.0066)
ν_{59}(0.1480)	0.0074(0.0013)	0.0157(0.0056)	-0.0017(0.0001)	0.0101(0.0023)	-0.0448(0.0458)	0.0002(0.0001)
ν_{64}(0.1574)	0.1447(0.4226)	0.0863(0.1503)	0.0782(0.1234)	0.0914(0.1686)	0.0381(0.0293)	0.0673(0.0914)
ν_{65}(0.1584)	0.0214(0.0091)	0.0537(0.0575)	0.0526(0.0551)	0.0446(0.0396)	0.0414(0.0342)	0.0004(0.0001)
ν_{67}(0.1694)	0.0145(0.0037)	-0.0176(0.0054)	-0.0379(0.0250)	-0.0089(0.0014)	0.0363(0.0230)	0.0145(0.0037)
ν_{68}(0.1718)	-0.0458(0.0355)	-0.0262(0.0116)	-0.0244(0.0101)	-0.0364(0.0224)	-0.0051(0.0004)	-0.0203(0.0070)
ν_{70}(0.1727)	-0.0809(0.1097)	-0.0080(0.0011)	0.0178(0.0053)	-0.0305(0.0156)	-0.0253(0.0107)	-0.0524(0.0460)
ν_{73}(0.1790)	0.0367(0.0210)	0.0300(0.0140)	0.0197(0.0061)	0.0383(0.0229)	0.0427(0.0285)	0.0609(0.0579)
ν_{76}(0.1829)	0.0012(0.0001)	0.0051(0.0004)	0.0119(0.0021)	0.0056(0.0005)	0.0030(0.0001)	0.0093(0.0013)
ν_{78}(0.1840)	-0.0118(0.0021)	-0.0127(0.0024)	-0.0209(0.0065)	-0.0103(0.0016)	0.0011(0.0001)	-0.0033(0.0002)
ν_{79}(0.1847)	-0.0161(0.0038)	0.0124(0.0023)	0.0046(0.0003)	0.0110(0.0018)	0.0056(0.0005)	-0.0131(0.0025)
ν_{82}(0.1926)	0.0637(0.0547)	0.0203(0.0056)	0.0288(0.0112)	0.0002(0.0001)	-0.0344(0.0160)	-0.0555(0.0415)
ν_{84}(0.2012)	0.0451(0.0251)	0.0292(0.0105)	0.0211(0.0055)	0.0323(0.0129)	0.0733(0.0664)	0.0245(0.0074)
ν_{86}(0.2065)	-0.2143(0.5385)	-0.0404(0.0191)	-0.0550(0.0355)	-0.0200(0.0047)	-0.1263(0.1870)	-0.0458(0.0246)
ν_{88}(0.2177)	-0.0181(0.0035)	-0.1323(0.1847)	-0.1994(0.4197)	-0.0758(0.0606)	-0.0102(0.0011)	-0.0140(0.0021)
ν_{90}(0.3765)	0.0021(0.0001)	0.0007(0.0001)	0.0027(0.0001)	0.0019(0.0001)	0.0023(0.0001)	0.0038(0.0001)
ν_{91}(0.3847)	0.0005(0.0001)	-0.0009(0.0001)	-0.0010(0.0001)	0.0002(0.0001)	-0.0011(0.0001)	-0.0009(0.0001)
ν_{94}(0.3889)	-0.0005(0.0001)	0.0079(0.0002)	0.0100(0.0003)	0.0025(0.0001)	-0.0003(0.0001)	-0.0005(0.0001)
ν_{95}(0.3922)	0.0046(0.0001)	0.0035(0.0001)	0.0016(0.0001)	0.0061(0.0001)	-0.0035(0.0001)	-0.0057(0.0001)
ν_{97}(0.3929)	-0.0082(0.0002)	-0.0052(0.0001)	-0.0022(0.0001)	-0.0074(0.0002)	-0.0168(0.0009)	0.0005(0.0001)
ν_{99}(0.3954)	0.0061(0.0001)	0.0010(0.0001)	-0.0004(0.0001)	0.0046(0.0001)	0.0033(0.0001)	0.0099(0.0003)
ν_{100}(0.3983)	-0.0021(0.0001)	-0.0020(0.0001)	-0.0028(0.0001)	0.0022(0.0001)	-0.0028(0.0001)	-0.0186(0.0011)
ν_{102}(0.3999)	-0.0025(0.0001)	0.0008(0.0001)	0.0016(0.0001)	-0.0017(0.0001)	-0.0138(0.0006)	-0.0051(0.0001)

Table S13: Linear interstate coupling parameters (λ) for triplet electronic states of **AP2** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

B mode (Freq, eV)	$\lambda_{T_1-T_2}$	$\lambda_{T_1-T_4}$	$\lambda_{T_1-T_5}$	$\lambda_{T_1-T_6}$	$\lambda_{T_2-T_3}$	$\lambda_{T_3-T_4}$	$\lambda_{T_3-T_5}$	$\lambda_{T_3-T_6}$
ν_2(0.0062)	-	-	0.0217(6.1250)	-	-	0.0157 (3.2062)	0.0368 (17.6150)	0.0353 (16.2082)
ν_4(0.0080)	0.0280(6.1250)	0.0377 (11.1038)	0.0283(6.2570)	0.0255 (5.0801)	-	0.0074 (0.4278)	0.0052 (0.2113)	-
ν_5(0.0156)	0.0243(1.2132)	0.0196 (0.7893)	-	-	-	0.0082(0.1381)	0.0126 (0.3262)	-
ν_8(0.0214)	0.0136(0.2019)	0.0201 (0.4411)	-	-	-	0.0079 (0.0681)	-	-
ν_9(0.0217)	0.0208(0.4594)	0.0508 (2.7402)	-	-	-	0.0158 (0.2651)	0.0159 (0.2684)	0.0152 (0.2453)
ν_{11}(0.0285)	0.0098(0.0591)	0.0224 (0.3089)	-	-	-	0.0076 (0.0356)	-	-
ν_{13}(0.0336)	0.0424(0.7962)	0.0530 (1.2441)	-	-	-	0.0114 (0.0576)	-	-
ν_{14}(0.0372)	-	0.0243 (0.2134)	-	-	0.0136 (0.0668)	-	-	-
ν_{16}(0.0429)	-	-	0.0237(0.1526)	-	0.0186 (0.0940)	-	-	-
ν_{19}(0.0538)	0.0118(0.0241)	0.0305 (0.1607)	0.0212(0.0776)	-	0.0124 (0.0266)	-	-	-
ν_{21}(0.0609)	0.0183(0.0451)	0.0220 (0.0653)	-	-	-	0.0058 (0.0045)	-	-
ν_{22}(0.0631)	0.0212(0.0564)	0.0249 (0.0779)	-	-	0.0042 (0.0022)	-	-	-
ν_{23}(0.0635)	0.0444(0.2444)	0.0462 (0.2647)	-	-	0.0078 (0.0075)	-	-	-
ν_{25}(0.0662)	0.0257(0.0754)	0.0445 (0.2259)	-	-	-	0.0100 (0.0114)	-	-
ν_{27}(0.0699)	-	0.0546 (0.3051)	0.0295(0.0891)	-	-	0.0247 (0.0624)	0.0386 (0.1525)	0.0361 (0.1334)
ν_{29}(0.0777)	-	0.0446 (0.1647)	-	-	0.0069 (0.0039)	0.0133 (0.0146)	0.0079 (0.0052)	0.0097 (0.0078)
ν_{31}(0.0810)	-	-	-	-	0.0103 (0.0081)	-	0.0062 (0.0029)	0.0083 (0.0052)
ν_{33}(0.0877)	0.0066(0.0028)	0.0335 (0.0730)	-	-	-	0.0097 (0.0061)	-	0.0105 (0.0072)
ν_{36}(0.0910)	-	-	-	-	0.0101 (0.0062)	-	-	-
ν_{37}(0.0956)	0.0437(0.1045)	0.0502 (0.1379)	0.0354(0.0686)	-	0.0065 (0.0023)	0.0017 (0.0002)	-	-
ν_{39}(0.1030)	0.0205(0.0198)	-	-	-	0.0118 (0.0066)	-	-	-
ν_{41}(0.1045)	-	0.0243 (0.0270)	0.0189(0.0164)	-	0.0279 (0.0356)	-	-	-
ν_{42}(0.1062)	0.0335(0.0498)	0.0313 (0.0434)	-	-	0.0096 (0.0041)	-	-	-
ν_{45}(0.1180)	-	0.0513 (0.0945)	-	-	0.0121 (0.0053)	0.0142 (0.0072)	-	-
ν_{47}(0.1216)	0.0402(0.0546)	0.0422 (0.0602)	-	-	0.0075 (0.0019)	-	-	-
ν_{49}(0.1231)	0.0381(0.0479)	0.0355 (0.0416)	-	-	0.0016 (0.0001)	-	-	-
ν_{50}(0.1239)	0.0218(0.0155)	-	-	-	-	0.0023 (0.0002)	-	-
ν_{51}(0.1263)	-	-	0.0142(0.0063)	0.0217(0.0148)	0.0124 (0.0048)	-	-	-
ν_{53}(0.1289)	-	-	0.0159(0.0076)	-	-	0.0109(0.0036)	0.0249(0.0187)	0.0234 (0.0165)
ν_{56}(0.1405)	0.0264(0.0177)	0.0366 (0.0339)	-	-	0.0036 (0.0003)	0.0039 (0.0004)	-	-
ν_{58}(0.1470)	-	0.0120 (0.0033)	-	0.0207 (0.0099)	-	0.0108 (0.0027)	-	0.0226 (0.0118)
ν_{60}(0.1488)	-	0.0459 (0.0476)	0.0242(0.0132)	-	-	0.0164 (0.0061)	0.0230 (0.0119)	0.0170 (0.0065)
ν_{61}(0.1502)	-	0.0616 (0.0841)	-	-	-	0.0288 (0.0184)	0.0413 (0.0378)	0.0202 (0.0090)
ν_{62}(0.1541)	-	0.0695 (0.1017)	-	-	0.0354 (0.0264)	0.0176 (0.0065)	-	-
ν_{63}(0.1556)	-	0.0630 (0.0820)	-	-	0.0217 (0.0097)	0.0178 (0.0065)	0.0116 (0.0028)	-
ν_{66}(0.1659)	-	0.0318 (0.0184)	-	0.0416 (0.0314)	-	0.0186 (0.0063)	0.0285 (0.0148)	0.0390 (0.0276)
ν_{69}(0.1719)	-	0.0384 (0.0250)	-	-	-	0.0155 (0.0041)	0.0215 (0.0078)	0.0217 (0.0080)
ν_{71}(0.1730)	0.0569(0.0541)	0.0830 (0.1151)	-	0.0468 (0.0366)	-	0.0212 (0.0075)	-	0.0168 (0.0047)
ν_{72}(0.1751)	0.0412(0.0277)	0.0536 (0.0469)	0.0524(0.0448)	0.0680 (0.0754)	0.0099 (0.0016)	0.0019 (0.0001)	-	0.0181 (0.0053)
ν_{74}(0.1793)	0.0242(0.0091)	0.0307 (0.0147)	0.0467(0.0339)	0.0426 (0.0282)	0.0062 (0.0006)	-	0.0141 (0.0031)	0.0102 (0.0016)
ν_{75}(0.1828)	-	0.0135 (0.0027)	0.0154(0.0035)	-	-	0.0053 (0.0004)	0.0099 (0.0015)	0.0093 (0.0013)
ν_{77}(0.1839)	-	0.0122 (0.0022)	0.0151(0.0034)	-	-	0.0061 (0.0006)	0.0114 (0.0019)	0.0132 (0.0026)
ν_{80}(0.1880)	0.0654(0.0605)	0.0806 (0.0919)	0.1248(0.2203)	0.0293 (0.0121)	0.0249 (0.0088)	-	0.0308 (0.0134)	-
ν_{81}(0.1909)	-	0.0817 (0.0916)	-	-	0.0283 (0.0110)	0.0141 (0.0027)	-	-
ν_{83}(0.2003)	0.0986(0.1212)	0.1374 (0.2353)	-	0.1064 (0.1411)	-	0.0230 (0.0066)	-	-
ν_{85}(0.2040)	0.0319(0.0122)	0.0357 (0.0153)	0.0487(0.0285)	-	0.0441 (0.0234)	-	-	-
ν_{87}(0.2172)	-	0.2133 (0.4822)	0.0375(0.0149)	-	0.0935 (0.0327)	0.0668 (0.0473)	0.0389 (0.0160)	0.0251 (0.0067)
ν_{89}(0.3765)	-	-	0.0212(0.0016)	-	-	0.0039 (0.0001)	0.0095 (0.0003)	0.0080 (0.0002)
ν_{92}(0.3847)	-	-	0.0181(0.0011)	-	-	0.0046 (0.0001)	0.0108 (0.0004)	0.0123 (0.0005)
ν_{93}(0.3889)	0.0118(0.0005)	0.0213 (0.0015)	-	-	0.0076 (0.0002)	-	-	-
ν_{96}(0.3927)	0.0086(0.0002)	0.0161 (0.0008)	0.0156(0.0008)	0.0241 (0.0019)	-	0.0023 (0.0001)	0.0022 (0.0001)	0.0080 (0.0002)
ν_{98}(0.3933)	0.0094(0.0003)	0.0135 (0.0006)	0.0174(0.0010)	0.0168 (0.0009)	0.0021 (0.0001)	0.0015 (0.0001)	0.0040 (0.0001)	0.0048 (0.0001)
ν_{101}(0.3999)	0.0070(0.0002)	0.0148 (0.0007)	-	0.0148(0.0007)	0.0022 (0.0001)	0.0023 (0.0001)	-	0.0042 (0.0001)

Table S14: Linear intrastate coupling parameters (κ) for singlet electronic states of **AP4** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

AG mode (Freq, eV)	κ^{S_1}	κ^{S_2}	κ^{S_3}	κ^{S_4}	κ^{S_5}	κ^{S_6}
ν_3(0.0065)	-0.0171(3.4605)	-0.0286(9.6800)	-0.0357(15.0846)	-0.0419(20.7720)	-0.0420(20.8525)	-0.0332(13.0098)
ν_7(0.0098)	-0.0080(0.3332)	-0.0035(0.0638)	-0.0089(0.4116)	-0.0042(0.0934)	-0.0014(0.0105)	-0.0041(0.0858)
ν_{10}(0.0179)	-0.0086(0.1154)	-0.0068(0.0722)	-0.0062(0.0606)	-0.0048(0.0360)	-0.0043(0.0294)	-0.0002(0.0001)
ν_{15}(0.0212)	-0.0019(0.0040)	0.0098(0.1068)	0.0110(0.1339)	0.0126(0.1768)	0.0124(0.1722)	0.0097(0.1053)
ν_{20}(0.0338)	-0.0033(0.0048)	-0.0005(0.0001)	0.0133(0.0778)	0.0217(0.2068)	0.0068(0.0203)	0.0034(0.0051)
ν_{22}(0.0343)	0.0131(0.0729)	-0.0011(0.0005)	0.0013(0.0007)	-0.0024(0.0024)	-0.0029(0.0035)	0.0093(0.0365)
ν_{29}(0.0482)	0.0233(0.1168)	0.0115(0.0285)	0.0187(0.0756)	0.0141(0.0425)	0.0113(0.0273)	0.0038(0.0030)
ν_{32}(0.0620)	0.0228(0.0676)	0.0118(0.0181)	0.0146(0.0278)	0.0173(0.0390)	0.0079(0.0081)	-0.0274(0.0975)
ν_{37}(0.0687)	-0.0116(0.0143)	-0.0001(0.0001)	0.0123(0.0160)	0.0205(0.0447)	0.0272(0.0782)	0.0072(0.0055)
ν_{40}(0.0733)	-0.0034(0.0011)	0.0140(0.0182)	0.0321(0.0962)	0.0312(0.0903)	0.0312(0.0909)	0.0007(0.0001)
ν_{45}(0.0830)	-0.0071(0.0037)	-0.0259(0.0487)	-0.0231(0.0387)	-0.0289(0.0608)	-0.0237(0.0409)	-0.0200(0.0290)
ν_{47}(0.0843)	0.0052(0.0019)	-0.0004(0.0001)	0.0056(0.0022)	0.0064(0.0028)	0.0046(0.0015)	0.0163(0.0188)
ν_{55}(0.1038)	0.0067(0.0021)	-0.0047(0.0010)	0.0031(0.0004)	0.0053(0.0013)	0.0122(0.0069)	0.0124(0.0071)
ν_{58}(0.1152)	-0.0003(0.0001)	-0.0117(0.0052)	-0.0002(0.0001)	-0.0118(0.0053)	-0.0039(0.0006)	-0.0168(0.0106)
ν_{62}(0.1222)	0.0024(0.0002)	0.0116(0.0045)	0.0149(0.0074)	0.0132(0.0059)	0.0214(0.0153)	0.0112(0.0042)
ν_{69}(0.1285)	-0.0185(0.0104)	-0.0134(0.0054)	-0.0148(0.0066)	-0.0117(0.0042)	-0.0036(0.0004)	0.0042(0.0005)
ν_{73}(0.1405)	0.0377(0.0360)	-0.0078(0.0015)	-0.0321(0.0261)	-0.0329(0.0273)	-0.0293(0.0218)	0.0060(0.0009)
ν_{77}(0.1497)	0.0100(0.0022)	0.0299(0.0199)	0.0215(0.0103)	0.0196(0.0086)	0.0195(0.0085)	0.0331(0.0244)
ν_{82}(0.1582)	-0.0994(0.1974)	-0.1051(0.2207)	-0.1074(0.2306)	-0.1203(0.2891)	-0.1223(0.2989)	-0.0982(0.1929)
ν_{85}(0.1698)	0.0406(0.0286)	0.0250(0.0108)	0.0102(0.0018)	-0.0096(0.0016)	-0.0025(0.0001)	0.0299(0.0155)
ν_{86}(0.1718)	0.0592(0.0594)	0.0438(0.0325)	0.0358(0.0217)	0.0478(0.0387)	0.0430(0.0314)	0.0610(0.0630)
ν_{91}(0.1723)	-0.0103(0.0018)	0.0162(0.0044)	0.0336(0.0190)	0.0361(0.0219)	0.0357(0.0215)	0.0032(0.0002)
ν_{98}(0.1830)	0.0032(0.0002)	-0.0042(0.0003)	-0.0085(0.0011)	-0.0111(0.0019)	-0.0094(0.0013)	-0.0048(0.0003)
ν_{102}(0.1841)	-0.0077(0.0009)	-0.0185(0.0050)	-0.0290(0.0124)	-0.0312(0.0144)	-0.0277(0.0113)	-0.0084(0.0010)
ν_{105}(0.1901)	0.0438(0.0265)	0.0084(0.0010)	0.0333(0.0153)	0.0293(0.0119)	0.0282(0.0110)	-0.0374(0.0194)
ν_{110}(0.2057)	0.1369(0.2215)	0.0685(0.0554)	0.0947(0.1060)	0.0912(0.0982)	0.1031(0.1256)	0.0226(0.0060)
ν_{114}(0.2183)	-0.0484(0.0246)	-0.0700(0.0514)	-0.0850(0.0757)	-0.1099(0.1267)	-0.1197(0.1504)	-0.0371(0.0144)
ν_{118}(0.3766)	0.0062(0.0001)	-0.0028(0.0001)	-0.0039(0.0001)	-0.0022(0.0001)	-0.0029(0.0001)	0.0015(0.0001)
ν_{121}(0.3848)	-0.0011(0.0001)	-0.0004(0.0001)	-0.0010(0.0001)	-0.0015(0.0001)	0.0004(0.0001)	-0.0009(0.0001)
ν_{126}(0.3890)	0.0010(0.0001)	-0.0060(0.0001)	-0.0068(0.0002)	-0.0064(0.0001)	-0.0068(0.0002)	-0.0001(0.0001)
ν_{128}(0.3984)	0.0023(0.0001)	0.0018(0.0001)	0.0004(0.0001)	0.0004(0.0001)	0.0016(0.0001)	0.0031(0.0001)
ν_{132}(0.4005)	-0.0036(0.0001)	-0.0013(0.0001)	0.0001(0.0001)	0.0003(0.0001)	-0.0005(0.0001)	-0.0042(0.0001)

Table S15: Linear interstate coupling parameters (λ) for singlet electronic states of **AP4** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

Vibrational mode (Freq, eV)	$\lambda_{S_1-S_2}$	$\lambda_{S_1-S_3}$	$\lambda_{S_1-S_4}$	$\lambda_{S_1-S_6}$	$\lambda_{S_2-S_3}$	$\lambda_{S_2-S_4}$	$\lambda_{S_2-S_5}$	$\lambda_{S_3-S_4}$	$\lambda_{S_3-S_5}$	$\lambda_{S_3-S_6}$	$\lambda_{S_4-S_5}$	$\lambda_{S_4-S_6}$	$\lambda_{S_5-S_6}$
ν_1(0.0037)	-	-	-	-	0.0014(0.0732)	-	-	-	-	-	0.0106(4.0958)	-	-
ν_2(0.0050)	-	-	-	-	-	-	-	-	0.0053(0.5535)	-	-	0.0097(1.8998)	-
ν_4(0.0065)	0.0087(0.8957)	-	-	0.0161(3.0718)	-	-	-	-	-	-	-	-	0.0060(0.4277)
ν_5(0.0067)	-	0.0096(1.0216)	-	-	-	-	-	-	-	-	-	0.0003(0.0011)	-
ν_6(0.0070)	-	-	-	-	-	-	-	-	-	-	0.0209(4.4734)	-	-
ν_8(0.0128)	0.0060(0.1099)	-	-	0.0297(2.6895)	-	-	-	0.0128(0.5021)	-	-	-	-	0.0115(0.4043)
ν_9(0.0131)	-	0.0067(0.1327)	-	-	-	-	-	-	0.0023(0.0148)	-	-	-	-
ν_{11}(0.0188)	-	-	-	-	-	-	-	-	-	0.0061(0.0526)	0.0026(0.0093)	-	-
ν_{12}(0.0190)	-	0.0102(0.1452)	-	-	-	-	-	-	-	-	-	0.0071(0.0701)	-
ν_{13}(0.0207)	-	-	-	-	0.0048(0.0268)	-	-	-	-	-	0.0111(0.1433)	-	-
ν_{14}(0.0207)	0.0061(0.0434)	-	-	0.0108(0.1361)	-	-	-	0.0096(0.1070)	-	-	-	-	0.0030(0.0104)
ν_{16}(0.0217)	-	-	-	-	-	-	-	-	0.0173(0.3160)	-	-	0.0187(0.3696)	-
ν_{17}(0.0242)	0.0051(0.0222)	-	-	0.0097(0.0796)	-	-	-	0.0077(0.0508)	-	-	-	-	0.0015(0.0018)
ν_{18}(0.0260)	-	-	-	-	0.0009(0.0006)	-	-	-	-	-	0.0081(0.0484)	-	-
ν_{19}(0.0299)	-	0.0129(0.0929)	-	-	-	-	-	-	0.0069(0.0263)	-	-	0.0189(0.2005)	-
ν_{21}(0.0343)	0.0087(0.0322)	-	-	0.0335(0.4782)	-	-	-	-	-	-	-	-	0.0125(0.0665)
ν_{23}(0.0378)	0.0176(0.1084)	-	-	0.0333(0.3871)	-	-	-	0.0114(0.0452)	-	-	-	-	0.0020(0.0014)
ν_{24}(0.0393)	-	0.0068(0.0151)	-	-	-	0.0079(0.0201)	-	-	0.0097(0.0303)	-	-	-	-
ν_{25}(0.0410)	-	-	-	-	0.0040(0.0046)	-	-	-	-	-	0.0049(0.0071)	-	-
ν_{26}(0.0432)	-	0.0208(0.1156)	-	-	-	0.0126(0.0427)	-	-	-	-	-	-	-
ν_{27}(0.0471)	-	-	0.0216(0.1050)	-	0.0100(0.0227)	-	-	-	-	-	0.0020(0.0009)	-	-
ν_{28}(0.0472)	0.0236(0.1250)	-	-	0.0393(0.3460)	-	-	-	0.0095(0.0204)	-	-	-	-	0.0051(0.0058)
ν_{30}(0.0574)	-	0.0224(0.0765)	-	-	-	0.0162(0.0397)	-	-	-	-	-	-	-
ν_{31}(0.0609)	-	-	-	-	0.0071(0.0068)	-	-	-	-	-	0.0181(0.0444)	-	-
ν_{33}(0.0632)	0.0122(0.0186)	-	-	0.0258(0.0831)	-	-	-	0.0088(0.0096)	-	-	-	-	0.0028(0.0010)
ν_{34}(0.0652)	0.0242(0.0689)	-	-	0.0450(0.2377)	-	-	-	-	-	-	-	-	0.0076(0.0068)
ν_{35}(0.0658)	-	-	-	-	-	-	-	-	0.0312(0.1123)	-	-	0.0227(0.0594)	-
ν_{36}(0.0673)	0.0036(0.0014)	-	-	0.0490(0.2648)	-	-	-	-	-	-	-	-	0.0192(0.0409)
ν_{38}(0.0712)	-	-	-	-	-	-	-	-	-	0.0182(0.0325)	0.0089(0.0078)	-	-
ν_{39}(0.0731)	-	-	-	0.0482(0.2175)	-	-	0.0207(0.0401)	-	-	-	-	-	0.0174(0.0284)
ν_{41}(0.0759)	-	0.0131(0.0149)	-	-	-	-	-	-	0.0043(0.0016)	-	-	0.0032(0.0009)	-
ν_{42}(0.0764)	-	-	-	-	0.0186(0.0297)	-	-	-	-	-	0.0188(0.0304)	-	-
ν_{43}(0.0813)	-	-	-	-	0.0120(0.0108)	-	-	-	-	0.0044(0.0014)	0.0286(0.0618)	-	-
ν_{44}(0.0817)	-	-	-	-	-	0.0031(0.0007)	-	-	0.0139(0.0146)	-	-	0.0057(0.0024)	
ν_{46}(0.0842)	-	-	-	0.0030(0.0006)	-	-	-	-	-	-	-	-	0.0079(0.0044)
ν_{48}(0.0881)	-	-	-	-	0.0162(0.0168)	-	-	-	-	-	0.0122(0.0096)	-	-
ν_{49}(0.0883)	0.0102(0.0067)	-	-	0.0295(0.0558)	-	-	-	0.0064(0.0026)	-	-	-	-	0.0105(0.0071)
ν_{50}(0.0909)	-	-	-	-	0.0072(0.0032)	-	-	-	-	-	0.0110(0.0073)	-	-
ν_{51}(0.0910)	-	-	-	-	-	0.0140(0.0118)	-	-	0.0068(0.0028)	-	-	-	-
ν_{52}(0.0943)	-	0.0044(0.0011)	-	-	-	0.0132(0.0099)	-	-	0.0105(0.0062)	-	-	0.0003(0.0001)	-
ν_{53}(0.1013)	0.0098(0.0047)	-	-	0.0088(0.0037)	-	-	0.0052(0.0013)	0.0068(0.0023)	-	-	-	-	-
ν_{54}(0.1032)	-	-	-	-	0.0132(0.0082)	-	-	-	-	-	0.0049(0.0011)	-	-
ν_{56}(0.1046)	-	0.0127(0.0074)	-	-	-	-	-	-	-	-	-	0.0011(0.0001)	-
ν_{57}(0.1098)	0.0090(0.0034)	-	-	0.0209(0.0181)	-	-	-	0.0184(0.0140)	-	-	-	-	0.0024(0.0002)
ν_{59}(0.1174)	-	0.0179(0.0116)	-	-	-	0.0095(0.0033)	-	-	-	-	-	-	-
ν_{60}(0.1194)	0.0106(0.0039)	-	-	0.0039(0.0005)	-	-	-	0.0138(0.0067)	-	-	-	-	-
ν_{61}(0.1210)	-	-	0.0173(0.0102)	-	0.0053(0.0010)	-	-	-	-	0.0063(0.0014)	-	-	-
ν_{63}(0.1228)	0.0135(0.0060)	-	-	0.0268(0.0239)	-	-	-	0.0058(0.0011)	-	-	-	-	0.0051(0.0009)
ν_{64}(0.1230)	-	-	-	-	0.0042(0.0006)	-	-	-	-	0.0079(0.0021)	0.0015(0.0001)	-	-
ν_{65}(0.1240)	-	0.0136(0.0060)	-	-	-	-	-	-	-	-	-	0.0037(0.0005)	-
ν_{66}(0.1249)	0.0187(0.0112)	-	-	0.0356(0.0406)	-	-	-	0.0111(0.0040)	-	-	-	-	0.0080(0.0021)
ν_{67}(0.1282)	-	-	-	-	0.0069(0.0014)	-	-	-	-	-	0.0016(0.0001)	-	-
ν_{68}(0.1283)	-	0.0039(0.0005)	-	-	-	0.0111(0.0038)	-	-	0.0125(0.0048)	-	-	0.0029(0.0003)	-
ν_{70}(0.1287)	-	0.0060(0.0011)	-	-	-	-	-	-	-	-	-	0.0040(0.0005)	-
ν_{71}(0.1289)	0.0050(0.0008)	-	-	0.0169(0.0086)	-	-	-	-	-	-	-	-	0.0079(0.0019)
ν_{72}(0.1339)	-	-	-	-	0.0138(0.0053)	-	-	-	-	0.0173(0.0083)	0.0238(0.0159)	-	-
ν_{74}(0.1412)	-	-	-	0.0174(0.0076)	-	-	0.0043(0.0005)	0.0169(0.0072)	-	-	-	-	0.0062(0.0010)
ν_{75}(0.1489)	-	-	-	-	-	-	-	-	0.0282(0.0179)	-	-	0.0180(0.0073)	-
ν_{76}(0.1492)	0.0059(0.0008)	-	-	0.0366(0.0302)	-	-	0.0166(0.0062)	0.0234(0.0123)	-	-	-	-	0.0116(0.0030)
ν_{78}(0.1506)	-	-	-	-	-	-	-	-	-	0.0109(0.0026)	0.0223(0.0110)	-	-
ν_{79}(0.1508)	-	-	-	-	-	-	-	-	0.0173(0.0066)	-	-	0.0160(0.0057)	-
ν_{80}(0.1544)	-	-	-	-	-	-	-	-	0.0504(0.0532)	-	-	0.0244(0.0125)	-

ν_{81}(0.1549)	-	-	-	0.0504(0.0530)	-	-	0.0422(0.0371)	0.0312(0.0203)	-	-	-	-	0.0111(0.0026)
ν_{83}(0.1592)	-	-	-	-	0.0289(0.0165)	-	-	-	-	0.0264(0.0138)	0.0489(0.0472)	-	-
ν_{84}(0.1658)	-	-	-	-	-	-	-	-	-	-	-	0.0097(0.0017)	-
ν_{87}(0.1718)	0.0239(0.0097)	-	-	0.0753(0.0962)	-	-	-	-	-	-	-	-	0.0248(0.0104)
ν_{88}(0.1720)	-	-	-	-	0.0217(0.0080)	-	-	-	-	-	0.0267(0.0121)	-	-
ν_{89}(0.1720)	-	-	-	0.0331(0.0185)	-	-	0.0201(0.0069)	0.0205(0.0071)	-	-	-	-	0.0114(0.0022)
ν_{90}(0.1721)	-	-	-	-	-	-	-	-	0.0297(0.0149)	-	-	0.0164(0.0045)	-
ν_{92}(0.1729)	-	0.0145(0.0035)	-	-	-	0.0116(0.0022)	-	-	-	-	-	0.0044(0.0003)	-
ν_{93}(0.1749)	-	-	-	-	0.0034(0.0002)	-	-	-	-	-	0.0242(0.0095)	-	-
ν_{94}(0.1775)	-	-	-	0.0126(0.0025)	-	-	-	0.0057(0.0005)	-	-	-	-	0.0048(0.0004)
ν_{95}(0.1827)	-	-	-	0.0104(0.0016)	-	-	-	0.0076(0.0009)	-	-	-	-	0.0061(0.0006)
ν_{96}(0.1828)	-	-	-	-	-	-	-	-	-	0.0024(0.0001)	0.0109(0.0018)	-	-
ν_{97}(0.1829)	-	-	-	-	-	-	-	-	0.0127(0.0024)	-	-	0.0077(0.0009)	-
ν_{99}(0.1840)	-	-	-	-	0.0065(0.0006)	-	-	-	-	-	0.0171(0.0043)	-	-
ν_{100}(0.1840)	-	-	-	0.0152(0.0034)	-	-	-	0.0142(0.0030)	-	-	-	-	0.0073(0.0008)
ν_{101}(0.1840)	-	-	-	-	-	-	-	-	0.0131(0.0026)	-	-	0.0084(0.0010)	-
ν_{103}(0.1851)	-	-	-	-	0.0179(0.0047)	-	-	-	-	-	0.0122(0.0022)	-	-
ν_{104}(0.1888)	-	-	-	-	-	-	-	-	0.0175(0.0043)	-	-	0.0103(0.0015)	-
ν_{106}(0.1908)	0.0005(0.0001)	-	-	0.0207(0.0059)	-	-	0.0186(0.0048)	0.0242(0.0080)	-	-	-	-	0.0022(0.0001)
ν_{107}(0.1971)	-	-	-	-	0.0182(0.0042)	-	-	-	-	-	0.0242(0.0075)	-	-
ν_{108}(0.1991)	0.0262(0.0087)	-	-	0.0772(0.0752)	-	-	-	-	-	-	-	-	0.0217(0.0059)
ν_{109}(0.2042)	-	0.0099(0.0012)	-	-	-	0.0192(0.0044)	-	-	0.0221(0.0059)	-	-	-	-
ν_{111}(0.2177)	0.0136(0.0020)	-	-	0.0549(0.0317)	-	-	0.0490(0.0254)	0.0519(0.0284)	-	-	-	-	-
ν_{112}(0.2177)	-	-	-	-	-	0.0170(0.0030)	-	-	0.0472(0.0235)	-	-	0.0259(0.0071)	-
ν_{113}(0.2179)	-	-	-	-	0.0432(0.0196)	-	-	-	-	0.0486(0.0249)	0.0672(0.0476)	-	-
ν_{115}(0.3766)	0.0023(0.0001)	-	-	0.0069(0.0002)	-	-	-	0.0043(0.0001)	-	-	-	-	0.0023(0.0001)
ν_{116}(0.3766)	-	-	-	-	0.0052(0.0001)	-	-	-	-	-	0.0057(0.0001)	-	-
ν_{117}(0.3766)	-	0.0056(0.0001)	-	-	-	0.0019(0.0001)	-	-	0.0040 (0.0001)	-	-	-	-
ν_{119}(0.3848)	-	-	0.0043(0.0001)	-	0.0003(0.0001)	-	-	-	-	-	0.0006 (0.0001)	-	-
ν_{120}(0.3848)	0.0024(0.0001)	-	-	0.0027(0.0001)	-	-	-	-	-	-	-	-	-
ν_{122}(0.3848)	-	0.0074(0.0002)	-	-	-	-	-	-	-	-	-	-	-
ν_{123}(0.3890)	0.0030(0.0001)	-	-	0.0051(0.0001)	-	-	0.0011(0.0001)	0.0073(0.0002)	-	-	-	-	-
ν_{124}(0.3890)	-	-	-	-	0.0078(0.0002)	-	-	-	-	-	0.0069(0.0002)	-	-
ν_{125}(0.3890)	-	0.0074(0.0002)	-	-	-	0.0079(0.0002)	-	-	0.0043(0.0001)	-	-	-	-
ν_{127}(0.3984)	-	-	-	-	-	-	-	-	-	0.0054(0.0001)	0.0014(0.0001)	-	-
ν_{129}(0.3984)	0.00(0.000)	-	-	-	-	-	-	0.0016(0.0001)	-	-	-	-	0.0025 (0.0001)
ν_{130}(0.3984)	-	-	-	-	-	-	-	-	-	0.0046(0.0001)	0.0012 (0.0001)	-	-
ν_{131}(0.4005)	-	-	-	-	-	0.0026(0.0001)	-	-	0.0003(0.0001)	-	-	0.0025(0.0001)	-

Table S16: Linear intrastate coupling parameters (κ) for triplet electronic states of **AP4** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\kappa^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

AG mode (Freq, eV)	κ^{T_1}	κ^{T_2}	κ^{T_3}	κ^{T_4}	κ^{T_5}	κ^{T_6}
ν_3(0.0065)	-0.0173(3.5567)	-0.0279(9.2053)	-0.0291(10.0145)	-0.0297(10.4659)	-0.0354(14.8680)	-0.0405(19.4491)
ν_7(0.0098)	-0.0030(0.0462)	0.0035(0.0647)	-0.0058(0.1762)	-0.0042(0.0935)	-0.0017(0.0159)	-0.0054(0.1505)
ν_{10}(0.0179)	-0.0096(0.1438)	-0.0071(0.0778)	-0.0044(0.0308)	-0.0016(0.0038)	-0.0008(0.0011)	-0.0015(0.0034)
ν_{15}(0.0212)	-0.0048(0.0256)	0.0087(0.0841)	0.0090(0.0909)	0.0098(0.1068)	0.0112(0.1396)	0.0103(0.1185)
ν_{20}(0.0338)	0.0115(0.0580)	-0.0152(0.1005)	0.0024(0.0026)	-0.0082(0.0298)	0.0074(0.0240)	0.0091(0.0361)
ν_{22}(0.0343)	0.0211(0.1898)	-0.0030(0.0038)	-0.0015(0.0010)	-0.0004(0.0001)	-0.0038(0.0061)	0.0069(0.0202)
ν_{29}(0.0482)	0.0289(0.1802)	0.0036(0.0028)	0.0142(0.0434)	0.0129(0.0359)	0.0075(0.0121)	0.0028(0.0017)
ν_{32}(0.0620)	0.0314(0.1286)	0.0029(0.0011)	0.0172(0.0387)	0.0178(0.0410)	0.0109(0.0154)	-0.0322(0.1347)
ν_{37}(0.0687)	-0.0118(0.0148)	-0.0101(0.0108)	0.0087(0.0080)	0.0085(0.0077)	0.0241(0.0614)	0.0150(0.0239)
ν_{40}(0.0733)	-0.0017(0.0003)	-0.0021(0.0004)	0.0204(0.0389)	0.0126 (0.0148)	0.0197(0.0361)	0.0093(0.0081)
ν_{45}(0.0830)	0.0024(0.0004)	-0.0239(0.0415)	-0.0247(0.0443)	-0.0311(0.0701)	-0.0269(0.0523)	-0.0145(0.0152)
ν_{47}(0.0843)	0.0076(0.0041)	-0.0014(0.0001)	0.0023(0.0004)	0.0040(0.0011)	0.0078(0.0043)	0.0212(0.0316)
ν_{55}(0.1038)	0.0166(0.0127)	-0.0066(0.0020)	0.0007(0.0001)	0.0019(0.0002)	0.0046(0.0010)	0.0115(0.0062)
ν_{58}(0.1152)	0.0092(0.0032)	-0.0305(0.0350)	-0.0061(0.0014)	-0.0124(0.0058)	-0.0096(0.0035)	-0.0175(0.0116)
ν_{62}(0.1222)	0.0029(0.0003)	0.0095(0.0030)	0.0084(0.0024)	0.0013(0.0001)	0.0117(0.0046)	0.0193(0.0125)
ν_{69}(0.1285)	-0.0185(0.0103)	-0.0126(0.0048)	-0.0172(0.0090)	-0.0186(0.0105)	-0.0074(0.0017)	0.0033(0.0003)
ν_{73}(0.1405)	0.0532(0.0717)	0.0104(0.0027)	-0.0234(0.0139)	-0.0147(0.0054)	-0.0293(0.0217)	-0.0119(0.0036)
ν_{77}(0.1497)	0.0131(0.0039)	0.0315(0.0221)	0.0181(0.0073)	0.0113(0.0029)	0.0155(0.0054)	0.0259(0.0150)
ν_{82}(0.1582)	-0.1426(0.4065)	-0.1051(0.2207)	-0.0920(0.1691)	-0.0857(0.1466)	-0.0976(0.1902)	-0.0988(0.1950)
ν_{85}(0.1698)	0.0689(0.0823)	0.0139(0.0034)	-0.0039(0.0003)	-0.0240(0.0100)	-0.0141(0.0035)	0.0165(0.0047)
ν_{86}(0.1718)	0.0762(0.0985)	0.0478(0.0386)	0.0280(0.0132)	0.0372(0.0234)	0.0306(0.0159)	0.0535(0.0486)
ν_{91}(0.1723)	-0.0132(0.0029)	0.0063(0.0007)	0.0260(0.0114)	0.0227(0.0087)	0.0286(0.0138)	0.0126(0.0027)
ν_{98}(0.1830)	0.0042(0.0003)	-0.0021(0.0001)	-0.0069(0.0007)	-0.0080(0.0010)	-0.0078(0.0009)	-0.0057(0.0005)
ν_{102}(0.1841)	-0.0080(0.0009)	-0.0116(0.0020)	-0.0216(0.0069)	-0.0208 (0.0064)	-0.0216(0.0069)	-0.0137(0.0028)
ν_{105}(0.1901)	0.0675(0.0630)	-0.0058(0.0005)	0.0270(0.0101)	0.0338(0.0158)	0.0221(0.0068)	-0.0141(0.0028)
ν_{110}(0.2057)	0.2153(0.5478)	0.0487(0.0281)	0.0778(0.0716)	0.0658(0.0511)	0.0752(0.0667)	0.0305(0.0110)
ν_{114}(0.2183)	-0.0222(0.0052)	-0.0814(0.0695)	-0.1162(0.1418)	-0.1411(0.2088)	-0.1324(0.1838)	-0.0624(0.0408)
ν_{118}(0.3766)	0.0020(0.0001)	-0.0001(0.0001)	-0.0011(0.0001)	0.0024(0.0001)	-0.0004(0.0001)	0.0006(0.0001)
ν_{121}(0.3848)	-0.0009(0.0001)	-0.0004(0.0001)	-0.0001(0.0001)	-0.0011(0.0001)	0.0001(0.0001)	-0.0010(0.0001)
ν_{126}(0.3890)	0.0009(0.0001)	-0.0044(0.0001)	-0.0073(0.0002)	-0.0052(0.0001)	-0.0077(0.0002)	-0.0018(0.0001)
ν_{128}(0.3984)	0.0024(0.0001)	-0.0001(0.0001)	0.0012(0.0001)	0.0018 (0.0001)	0.0020(0.0001)	-0.0028(0.0001)
ν_{132}(0.4005)	-0.0044(0.0001)	-0.0026(0.0001)	0.0005(0.0001)	0.0001(0.0001)	0.0003(0.0001)	-0.0035(0.0001)

Table S17: Linear interstate coupling parameters (λ) for triplet electronic states of **AP4** obtained at B3LYP/6-311G(d,p) level of theory. Coupling strength ($\lambda^2/2\omega^2$) obtained for each vibrational mode is shown in paranthesis.

Vibrational mode (Freq, eV)	$\lambda_{T_1-T_2}$	$\lambda_{T_1-T_3}$	$\lambda_{T_1-T_4}$	$\lambda_{T_1-T_6}$	$\lambda_{T_2-T_3}$	$\lambda_{T_2-T_4}$	$\lambda_{T_2-T_5}$	$\lambda_{T_3-T_4}$	$\lambda_{T_3-T_5}$	$\lambda_{T_3-T_6}$	$\lambda_{T_4-T_5}$	$\lambda_{T_4-T_6}$	$\lambda_{T_5-T_6}$
ν_1(0.0037)	-	-	-	-	-	-	-	-	-	-	0.0091 (3.0245)	-	-
ν_2(0.0050)	-	-	-	-	-	-	-	-	0.0092(1.6928)	-	-	0.0111 (2.4642)	-
ν_4(0.0065)	-	-	-	-	-	-	-	0.0069 (0.5634)	-	-	-	-	0.0116 (1.5924)
ν_5(0.0067)	-	-	-	-	-	-	-	-	0.0027(0.0812)	-	-	-	-
ν_6(0.0070)	-	-	-	-	-	-	-	-	-	-	0.0163 (2.7111)	-	-
ν_8(0.0128)	0.0251(1.9226)	-	-	0.0567 (9.8111)	-	-	-	0.0115 (0.4036)	-	-	-	-	0.0163 (0.8108)
ν_9(0.0131)	-	0.0190(1.0518)	-	-	-	-	-	-	-	-	-	-	-
ν_{11}(0.0188)	-	-	-	-	0.0052 (0.0383)	-	-	-	-	0.0060(0.0509)	0.0022 (0.0068)	-	-
ν_{12}(0.0190)	-	0.0200(0.5540)	-	-	-	-	-	-	-	-	-	0.0083 (0.0954)	-
ν_{13}(0.0207)	-	-	-	-	-	-	-	-	-	0.0017(0.0034)	0.0084 (0.0823)	-	-
ν_{14}(0.0207)	0.0156(0.2840)	-	-	0.0237 (0.6554)	-	-	-	0.0050 (0.0292)	-	-	-	-	0.0072 (0.0605)
ν_{16}(0.0217)	-	-	-	-	-	-	-	-	0.0153(0.2486)	-	-	0.0167 (0.2961)	-
ν_{17}(0.0242)	0.0136(0.1579)	-	-	0.0108 (0.0996)	-	-	-	0.0026 (0.0058)	-	-	-	-	0.0014 (0.0017)
ν_{18}(0.0260)	-	-	0.0305(0.6881)	-	0.0069 (0.0352)	-	-	-	-	0.0022(0.0036)	-	-	-
ν_{19}(0.0299)	-	0.0203(0.2305)	-	-	-	-	-	-	0.0070(0.0274)	-	-	0.0175 (0.1713)	-
ν_{21}(0.0343)	0.0354(0.5326)	-	-	0.0652 (1.8067)	-	-	-	0.0070 (0.0208)	-	-	-	-	0.0155 (0.1021)
ν_{23}(0.0378)	-	-	-	0.0211 (0.1558)	-	-	0.0150(0.0787)	0.0128 (0.0573)	-	-	-	-	0.0023 (0.0019)
ν_{24}(0.0393)	-	0.0227(0.1668)	-	-	-	0.0042 (0.0057)	-	-	0.0055(0.0098)	-	-	-	-
ν_{25}(0.0410)	-	-	-	-	0.0086 (0.0220)	-	-	-	-	-	0.0045 (0.0060)	-	-
ν_{26}(0.0432)	-	0.0190(0.0967)	-	-	-	0.0224 (0.1344)	-	-	0.0110(0.0324)	-	-	-	-
ν_{27}(0.0471)	-	-	0.0162(0.0592)	-	0.0195 (0.0857)	-	-	-	-	-	0.0088 (0.0175)	-	-
ν_{28}(0.0472)	0.0293(0.1927)	-	-	0.0204 (0.0934)	-	-	-	0.0194 (0.0845)	-	-	-	-	-
ν_{30}(0.0574)	-	0.0293(0.1303)	-	-	-	0.0166 (0.0418)	-	-	-	-	-	-	-
ν_{31}(0.0609)	-	-	-	-	0.0080 (0.0086)	-	-	-	-	-	0.0137 (0.0253)	-	-
ν_{33}(0.0632)	0.0291(0.1060)	-	-	0.0453 (0.2569)	-	-	-	0.0039 (0.0019)	-	-	-	-	0.0073 (0.0067)
ν_{34}(0.0652)	0.0424(0.2114)	-	-	0.0561 (0.3702)	-	-	-	0.0103 (0.0125)	-	-	-	-	0.0060 (0.0042)
ν_{35}(0.0658)	-	-	-	-	-	-	-	-	0.0219(0.0554)	-	-	0.0198 (0.0453)	-
ν_{36}(0.0673)	0.0083(0.0076)	-	-	0.0663 (0.4853)	-	-	-	0.0043 (0.0020)	-	-	-	-	0.0207 (0.0473)
ν_{38}(0.0712)	-	-	-	-	-	-	-	-	-	0.0148(0.0216)	0.0015 (0.0002)	-	-
ν_{39}(0.0731)	-	-	-	0.0895 (0.7495)	-	-	-	0.0177 (0.0293)	-	-	-	-	0.0278 (0.0723)
ν_{41}(0.0759)	-	-	-	-	-	0.0055 (0.0026)	-	-	-	-	-	-	-
ν_{42}(0.0764)	-	-	-	-	0.0200 (0.0343)	-	-	-	-	-	0.0152 (0.0198)	-	-
ν_{43}(0.0813)	-	-	-	-	-	-	-	-	-	0.0169(0.0216)	0.0254 (0.0488)	-	-
ν_{44}(0.0817)	-	-	-	-	-	-	-	-	0.0191(0.0273)	-	-	0.0104 (0.0081)	-
ν_{46}(0.0842)	-	-	-	-	-	-	0.0140(0.0138)	-	-	-	-	-	-
ν_{48}(0.0881)	-	-	-	-	0.0187 (0.0225)	-	-	-	-	-	0.0137 (0.0121)	-	-
ν_{49}(0.0883)	0.0159(0.0162)	-	-	0.0508 (0.1655)	-	-	-	0.0100 (0.0064)	-	-	-	-	0.0137 (0.0120)
ν_{50}(0.0909)	-	-	0.0343(0.0712)	-	0.0123 (0.0092)	-	-	-	-	-	0.0062 (0.0023)	-	-
ν_{51}(0.0910)	-	0.0172(0.0179)	-	-	-	0.0166 (0.0166)	-	-	0.0015(0.0001)	-	-	-	-
ν_{52}(0.0943)	-	-	-	-	-	0.0202 (0.0229)	-	-	0.0163(0.0149)	-	-	-	-
ν_{53}(0.1013)	0.0146(0.0104)	-	-	0.0131 (0.0084)	-	-	0.0175(0.0149)	-	-	-	-	-	-
ν_{54}(0.1032)	-	-	0.0346(0.0562)	-	0.0121 (0.0069)	-	-	-	-	-	0.0013 (0.0001)	-	-
ν_{56}(0.1046)	-	0.0324(0.0480)	-	-	-	0.0108 (0.0053)	-	-	0.0017(0.0001)	-	-	-	-
ν_{57}(0.1098)	-	-	-	0.0372 (0.0574)	-	-	0.0122(0.0062)	0.0294 (0.0358)	-	-	-	-	0.0090 (0.0034)
ν_{59}(0.1174)	-	-	-	-	-	-	-	-	0.0190(0.0131)	-	-	0.0165 (0.0099)	-
ν_{60}(0.1194)	0.0080(0.0022)	-	-	0.0361 (0.0457)	-	-	-	0.0127 (0.0057)	-	-	-	-	0.0104 (0.0038)
ν_{61}(0.1210)	-	-	-	-	0.0129 (0.0057)	-	-	-	-	-	0.0071 (0.0017)	-	-
ν_{63}(0.1228)	0.0393(0.0512)	-	-	0.0481 (0.0767)	-	-	0.0059(0.0012)	0.0059 (0.0012)	-	-	-	-	-
ν_{64}(0.1230)	-	-	0.0432(0.0617)	-	0.0082 (0.0022)	-	-	-	-	-	-	-	-
ν_{65}(0.1240)	-	0.0109(0.0039)	-	-	-	-	-	-	-	-	-	0.0095 (0.0029)	-
ν_{66}(0.1249)	0.0197(0.0124)	-	-	0.0218 (0.0152)	-	-	-	0.0109 (0.0038)	-	-	-	-	0.0061 (0.0012)
ν_{67}(0.1282)	-	-	-	-	0.0124 (0.0047)	-	-	-	-	-	0.0091 (0.0025)	-	-
ν_{68}(0.1283)	-	0.0144(0.0063)	-	-	-	0.0126 (0.0048)	-	-	0.0065(0.0013)	-	-	-	-
ν_{70}(0.1287)	-	-	-	-	-	-	-	-	-	-	-	0.0033 (0.0003)	-
ν_{71}(0.1289)	-	-	-	0.0081 (0.0020)	-	-	-	0.0051 (0.0008)	-	-	-	-	0.0074 (0.0016)
ν_{72}(0.1339)	-	-	-	-	-	-	-	-	-	0.0258(0.0186)	0.0164 (0.0075)	-	-
ν_{74}(0.1412)	0.0190(0.0091)	-	-	0.0342 (0.0293)	-	-	-	0.0091 (0.0021)	-	-	-	-	0.0074 (0.0014)
ν_{75}(0.1489)	-	-	-	-	-	-	-	-	0.0263(0.0156)	-	-	0.0244 (0.0134)	-
ν_{76}(0.1492)	-	-	-	0.0708 (0.1126)	-	-	-	0.0226 (0.0115)	-	-	-	-	0.0227 (0.0116)
ν_{78}(0.1506)	-	-	-	-	-	-	-	-	-	0.0114(0.0029)	0.0193 (0.0082)	-	-
ν_{79}(0.1508)	-	-	-	-	-	-	-	-	0.0144(0.0046)	-	-	0.0274 (0.0165)	-
ν_{80}(0.1544)	-	-	-	-	-	0.0237 (0.0118)	-	-	0.0511(0.0548)	-	-	0.0154 (0.0050)	-

ν_{81}(0.1549)	-	-	-	0.1146 (0.2737)	-	-	-	0.0440 (0.0403)	-	-	-	-	0.0319 (0.0212)
ν_{83}(0.5920)	-	-	-	-	0.0369 (0.0019)	-	-	-	-	-	0.0466 (0.0031)	-	-
ν_{84}(0.1658)	-	-	-	-	-	-	-	-	-	-	-	0.0128 (0.0030)	-
ν_{87}(0.1718)	0.0609(0.0628)	-	-	0.0992 (0.1667)	-	-	-	-	-	-	-	-	0.0257 (0.0112)
ν_{88}(0.1720)	-	-	-	-	-	-	-	-	-	0.0103(0.0018)	0.0141 (0.0034)	-	-
ν_{89}(0.1720)	-	-	-	0.0462 (0.0361)	-	-	-	0.0136 (0.0031)	-	-	-	-	0.0146 (0.0036)
ν_{90}(0.1721)	-	-	-	-	-	-	-	-	0.0189(0.0060)	-	-	0.0136 (0.0031)	-
ν_{92}(0.1729)	-	0.0596(0.0594)	-	-	-	0.0194 (0.0063)	-	-	0.0059(0.0006)	-	-	-	-
ν_{93}(0.1749)	-	-	-	-	0.0131 (0.0028)	-	-	-	-	-	0.0228 (0.0085)	-	-
ν_{94}(0.1775)	0.0130(0.0027)	-	-	0.0402 (0.0256)	-	-	-	0.0071 (0.0008)	-	-	-	-	0.0106 (0.0018)
ν_{95}(0.1827)	-	-	-	0.0028 (0.0001)	-	-	-	0.0027 (0.0001)	-	-	-	-	0.0038 (0.0002)
ν_{96}(0.1828)	-	-	-	-	-	-	-	-	-	-	0.0090 (0.0012)	-	-
ν_{97}(0.1829)	-	-	-	-	-	-	-	-	0.0071(0.0008)	-	-	0.0084 (0.0011)	-
ν_{99}(0.1840)	-	-	-	-	-	-	-	-	-	-	0.0127 (0.0024)	-	-
ν_{100}(0.1840)	-	-	-	0.0163 (0.0039)	-	-	-	0.0055 (0.0004)	-	-	-	-	0.0072 (0.0008)
ν_{101}(0.1840)	-	-	-	-	-	-	-	-	0.0063(0.0006)	-	-	0.0074 (0.0008)	-
ν_{103}(0.1851)	-	-	-	-	0.0213 (0.0066)	-	-	-	-	-	0.0076 (0.0008)	-	-
ν_{104}(0.1888)	-	0.0561(0.0441)	-	-	-	0.0317 (0.0141)	-	-	0.0298(0.0125)	-	-	-	-
ν_{106}(0.1908)	0.0214(0.0063)	-	-	0.0730 (0.0732)	-	-	-	0.0307 (0.0129)	-	-	-	-	0.0153 (0.0032)
ν_{107}(0.1971)	-	-	0.0506(0.0330)	-	0.0202 (0.0053)	-	-	-	-	-	0.0189 (0.0046)	-	-
ν_{108}(0.1991)	0.1090(0.1499)	-	-	0.1571 (0.3113)	-	-	-	0.0417 (0.0219)	-	-	-	-	0.0318 (0.0128)
ν_{109}(0.2042)	-	0.0459(0.0253)	-	-	-	0.0489 (0.0287)	-	-	0.0351(0.0148)	-	-	-	-
ν_{111}(0.2177)	-	-	-	0.1703 (0.3060)	-	-	0.0834(0.0734)	0.0812 (0.0696)	-	-	-	-	0.0318 (0.0128)
ν_{112}(0.2177)	-	-	-	-	-	-	-	-	0.0962(0.0976)	-	-	0.0578(0.0352)	-
ν_{113}(0.2179)	-	-	-	-	0.0450 (0.0213)	-	-	-	-	0.0593(0.0370)	0.0993 (0.1038)	-	-
ν_{115}(0.3766)	-	-	-	-	-	-	-	-	-	-	-	-	0.0015 (0.0001)
ν_{116}(0.3766)	-	-	-	-	0.0025 (0.0001)	-	-	-	-	0.0003(0.0001)	0.0017 (0.0001)	-	-
ν_{117}(0.3766)	-	0.0099(0.0003)	-	-	-	-	-	-	-	-	-	0.0039(0.0001)	-
ν_{119}(0.3848)	-	-	-	-	0.0032 (0.0001)	-	-	-	-	0.0009(0.0001)	0.0022 (0.0001)	-	-
ν_{120}(0.3848)	-	-	-	-	-	-	-	-	-	-	-	-	0.0015 (0.0001)
ν_{122}(0.3848)	-	0.0099(0.0003)	-	-	-	-	-	-	-	-	-	0.0044 (0.0001)	-
ν_{123}(0.3890)	-	-	-	0.0127 (0.0005)	-	-	0.0030(0.0001)	0.0039 (0.0001)	-	-	-	-	0.0026 (0.0001)
ν_{124}(0.3890)	-	-	-	-	0.0093 (0.0003)	-	-	-	-	-	0.0068 (0.0002)	-	-
ν_{125}(0.3890)	-	0.0137(0.0006)	-	-	-	0.0073 (0.0002)	-	-	0.0067(0.0001)	-	-	-	-
ν_{127}(0.3984)	-	-	-	-	-	-	-	-	-	0.0049(0.0001)	0.0029 (0.0001)	-	-
ν_{129}(0.3984)	-	-	-	0.0011 (0.0001)	-	-	0.0055(0.0001)	0.0010 (0.0001)	-	-	-	-	0.0016 (0.0001)
ν_{130}(0.3984)	-	-	-	-	0.0042 (0.0001)	-	-	-	-	0.0033(0.0001)	0.0017 (0.0001)	-	-
ν_{131}(0.4005)	-	0.0152(0.0007)	-	-	-	0.0039 (0.0001)	-	-	-	-	-	0.0024 (0.0001)	-

Fig. S2: Adiabatic potential energy curves of singlet electronic states along the dimensionless normal coordinates of C=C stretch vibration (Q_{51}) for **P**, C=O stretch vibration (Q_{88}) for **AP2** and C=O stretch vibration (Q_{114}) for **AP4**. Computed energies (plus harmonic potential) are shown by the asterisks on each curve.

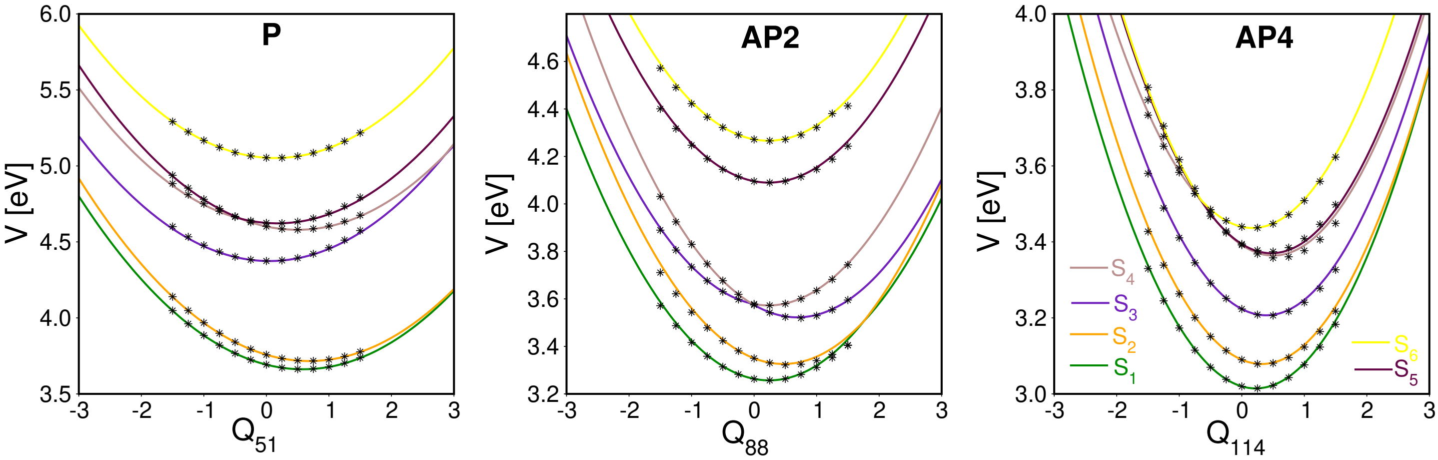

Fig. S3: Potential energy surfaces of triplet manifold and S_1 along the dimensionless normal coordinates of C=C stretch vibration (Q_{86}) and C=O stretch vibration (Q_{88}) of **AP2**.

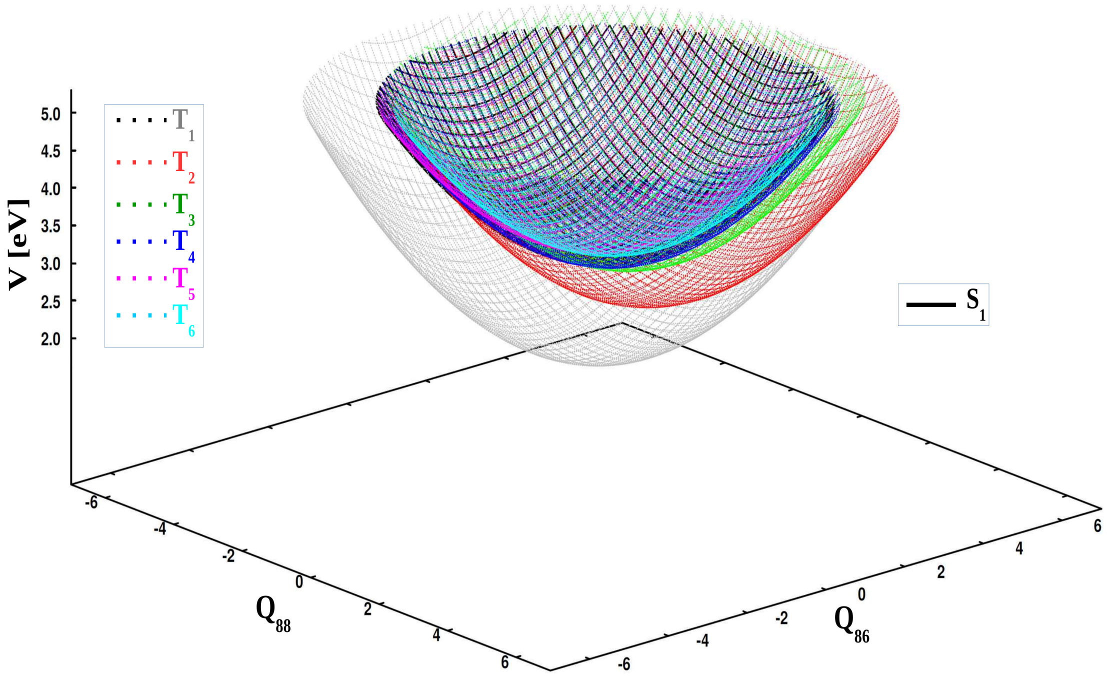

Fig. S4: Potential energy surfaces of triplet manifold and S_1 along the dimensionless normal coordinates of C=C stretch vibration (Q_{105}) and C=O stretch vibration (Q_{114}) of **AP4**.

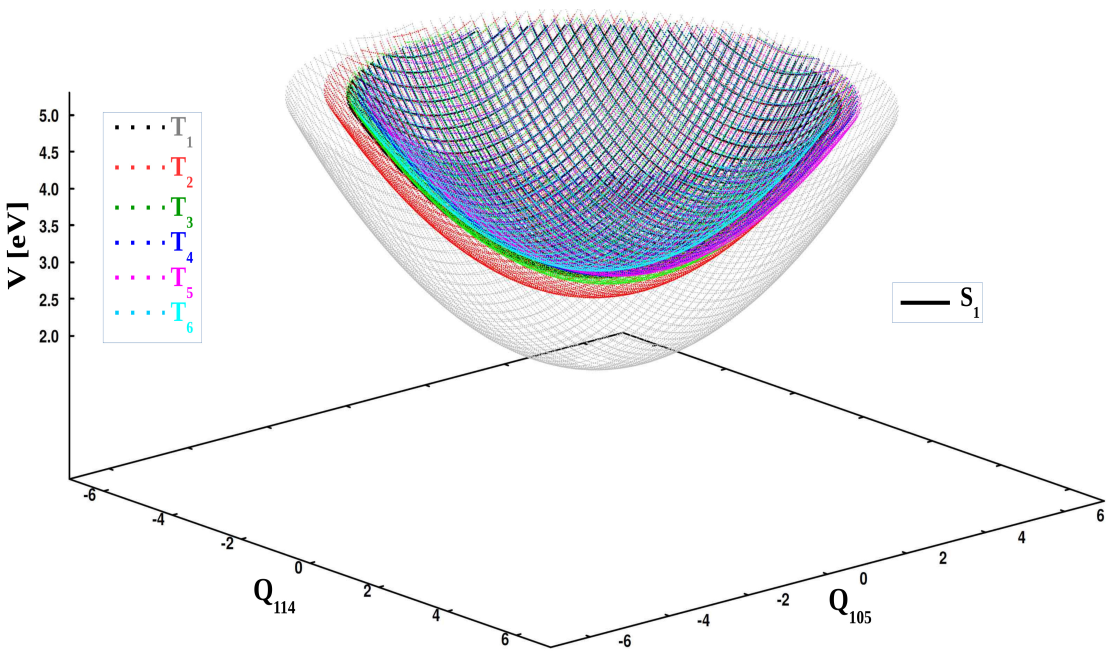

Fig. S5: Electronic population decay profiles of singlet manifold of **P**, **AP2** and **AP4**. The initial MCTDH wavepacket is placed on the FC point of individual electronic state of respective molecule and its time-evolution is monitored.

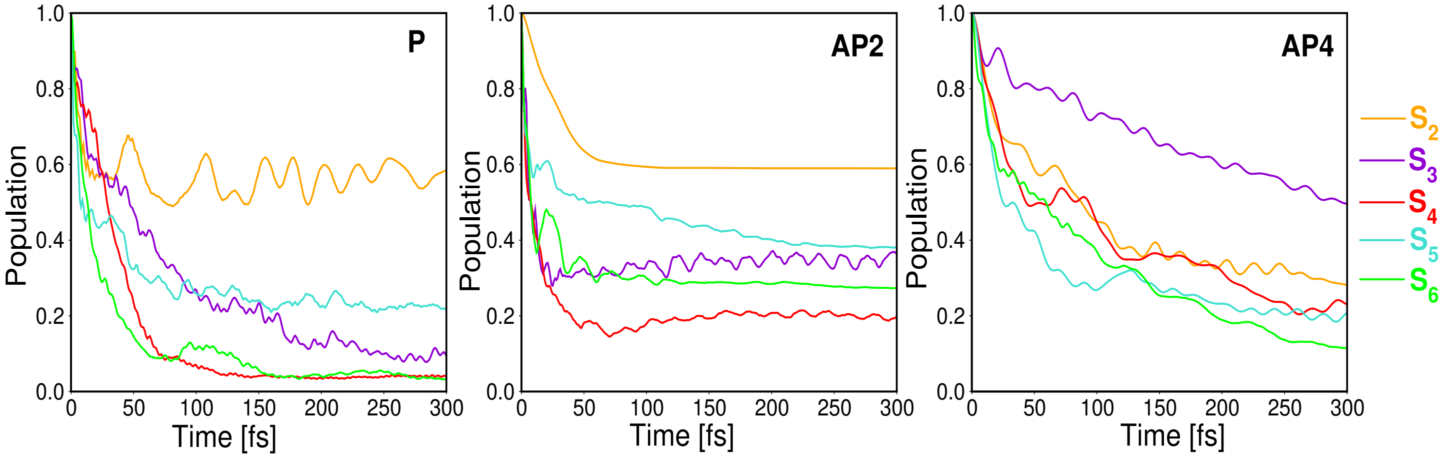

Fig. S6: Initial electronic populatian decay profile of S_2 state of **P**. The initial MCTDH wavepacket is placed on the FC point of S_2 electronic state and its time-evolution is monitored. The S_2 state lifetime is calculated by fitting the initial electronic population (shown in black) to a simple monoexponential function.

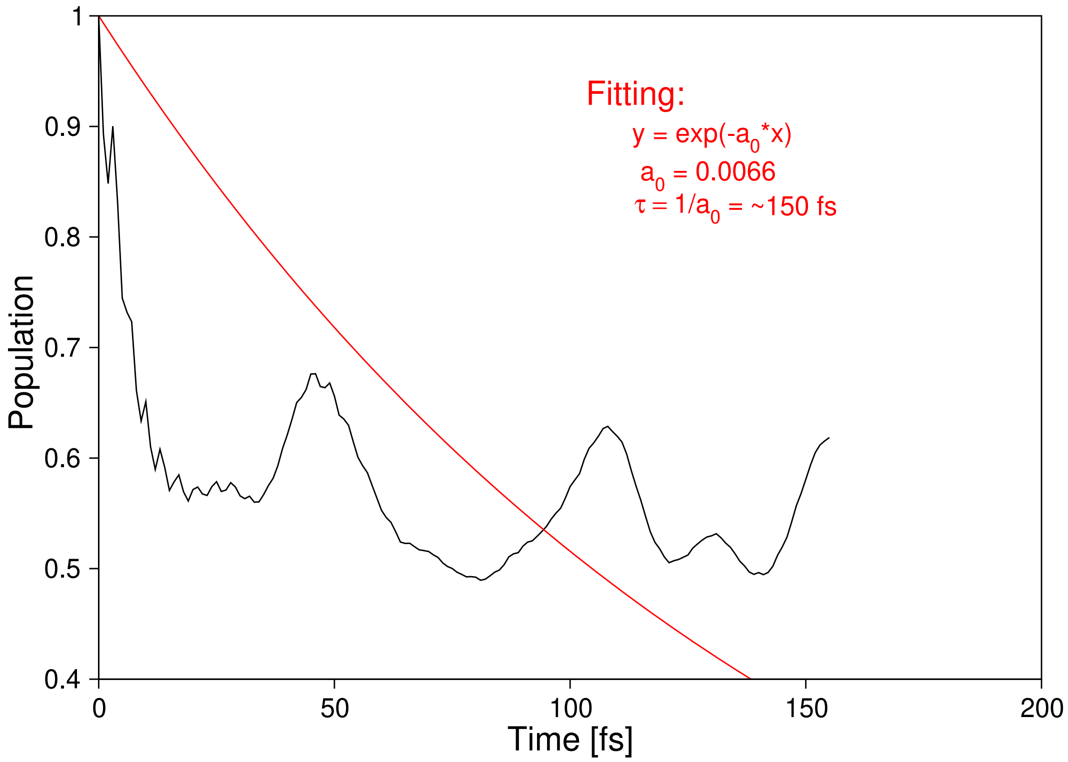

Table S18: MCTDH details of normal mode combination, primitive basis and single particle basis used in the S_1-S_6 dynamics and T_1-T_4 / T_1-T_5 dynamics of **P**, **AP2** and **AP4**.

Singlets			
	Normal modes	**Primitive basis**	**SPF basis**
	(ν_3,ν_{11},ν_{16},ν_{23},ν_{26})	(7,9,7,5,4)	[4,4,4,4,7,4]
	(ν_1,ν_9,ν_{13},ν_{19},ν_{27})	(10,9,6,8,4)	[7,4,5,5,10,6]
P	(ν_4,ν_7,ν_{15},ν_{24},ν_{29})	(5,7,7,7,6)	[4,4,4,4,7,5]
	(ν_2,ν_8,ν_{18},ν_{21},ν_{30})	(6,7,8,4,7)	[6,7,4,6,4,4]
	(ν_6,ν_{12},ν_{14},ν_{20},ν_{28})	(7,8,6,4,4)	[7,6,4,5,5,6]
	(ν_5,ν_{10},ν_{17},ν_{22},ν_{25})	(6,6,6,6,5)	[4,4,6,4,4,4]
	(ν_3,ν_{10},ν_{14},ν_{21},ν_{28})	(7,7,8,7,6)	[4,5,6,4,4,4]
	(ν_4,ν_{11},ν_{16},ν_{23},ν_{27})	(6,10,9,9,7)	[4,4,4,4,5,5]
	(ν_1,ν_2,ν_{26},ν_{22})	(10,9,6,8)	[8,9,10,9,8,7]
AP2	(ν_8,ν_{12},ν_{17},ν_{30})	(7,10,9,7)	[5,5,5,5,4,4]
	(ν_5,ν_{15},ν_{19},ν_{20})	(5,9,8,7)	[4,4,4,4,5,5]
	(ν_9,ν_{13},ν_{18},ν_{24})	(8,9,8,8)	[5,4,4,4,5,5]
	(ν_6,ν_7,ν_{25},ν_{29})	(6,6,6,7)	[4,4,4,4,5,5]
	(ν_3,ν_{11},ν_{16},ν_{23},ν_{26})	(6,9,6,7,5)	[4,5,5,5,5,5]
	(ν_1,ν_9,ν_{13},ν_{19},ν_{27})	(10,6,4,8,9)	[7,8,10,10,10,9]
AP4	(ν_4,ν_7,ν_{15},ν_{24},ν_{29})	(5,6,7,6,5)	[5,6,6,6,6,5]
	(ν_2,ν_8,ν_{18},ν_{21},ν_{30})	(7,6,6,5,5)	[7,4,7,4,4,4]
	(ν_6,ν_{12},ν_{14},ν_{20},ν_{28})	(4,5,7,9,9)	[4,4,4,4,4,4]
	(ν_5,ν_{10},ν_{17},ν_{22},ν_{25})	(5,9,6,5,5)	[5,4,4,4,4,4]
Triplets			
	(ν_1,ν_{11},ν_{14},ν_{21},ν_{30})	(9,4,4,7,8)	[8,4,4,7]
	(ν_2,ν_8,ν_{16},ν_{23},ν_{28})	(6,5,5,6,5)	[4,5,6,6]
P	(ν_3,ν_7,ν_9,ν_{22},ν_{25})	(5,7,10,5,5)	[9,6,9,7]
	(ν_4,ν_{12},ν_{13},ν_{17},ν_{27})	(7,4,4,4,4)	[5,4,6,4]
	(ν_6,ν_{15},ν_{19},ν_{20},ν_{26})	(5,4,5,5,5)	[4,4,5,4]
	(ν_5,ν_{10},ν_{18},ν_{24},ν_{29})	(8,4,7,7,4)	[8,6,4,6]
	(ν_3,ν_8,ν_{14},ν_{21},ν_{28})	(4,5,10,5,4)	[4,4,4,5]
	(ν_4,ν_{11},ν_{16},ν_{23},ν_{27})	(5,8,8,6,5)	[7,5,6,6]
	(ν_1,ν_7,ν_{10},ν_{26},ν_{22})	(10,4,6,6,7)	[8,9,10,10]
AP2	(ν_2,ν_6,ν_{12},ν_{17},ν_{30})	(9,6,7,9,7)	[7,7,8,8]
	(ν_5,ν_{15},ν_{19},ν_{20},ν_{25})	(6,9,9,6,5)	[6,4,4,4]
	(ν_9,ν_{13},ν_{18},ν_{24},ν_{29})	(5,10,8,6,6)	[4,4,5,4]
	(ν_3,ν_{11},ν_{16},ν_{23},ν_{26})	(5,8,4,5,4)	[5,4,4,4,4,]
	(ν_1,ν_9,ν_{13},ν_{19},ν_{27})	(10,9,6,8,7)	[8,9,9,9,10]
	(ν_4,ν_7,ν_{15},ν_{24},ν_{29})	(5,6,6,9,4)	[4,5,6,6,7]
AP4	(ν_2,ν_8,ν_{18},ν_{21},ν_{30})	(5,7,8,7,5)	[4,4,5,4,4]
	(ν_6,ν_{12},ν_{14},ν_{20},ν_{28})	(7,4,7,7,4)	[7,4,4,4,4]
	(ν_5,ν_{10},ν_{17},ν_{22},ν_{25})	(7,7,8,6,9)	[7,6,5,5,5]