Electronic Supplementary Material (ESI) for Journal of Materials Chemistry
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SUPPORTING INFORMATION

Liaisons Between Photoconductivity and Molecular Frame in Organometallic Pd(II) and Pt(II) Complexes

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SI-1. Experimental

General

Reagents were used as supplied from Sigma-Aldrich. Spectrofluorimetric grade dichloromethane (Acros Organics) were used for the photophysical investigations in solution, at room temperature.

^{1}H NMR spectra were acquired on a Bruker Advance DRX-300 spectrometer in $CDCl_3$ solution, with TMS as internal standard. Infrared spectra were recorded with a Spectrum One FT-IR Perkin-Elmer spectrometer. Elemental analyses were performed with a Perkin-Elmer 2400 microanalyzer by the Microanalytical Laboratory at University of Calabria. The thermal behaviour of all complexes was studied with a Zeiss Axioscope polarizing microscope equipped with a Linkam CO 600 heating stage.

SI-2. Synthesis

The azobenzene cycloplatinated derivative, parent of **AZPtON,** was prepared from allyl platinum [1] whereas the Pt(II) chloride bridged dimers, precusors of **PYPtON**, and **BEPtON**, were obtained by microwave assisted reactions from the reaction of the platinum salt (K_2PtCl_4) with the corresponding ligand; their syntheses are fully described in our previous work [2].

*General procedure for complexes **AZPtON**, **PYPtON** and **BEPtON**.*

To a stirred solution of the adequate Pt(II) chloride bridged dimer (500 mg) in degassed (N_2) 2-ethoxyethanol (50 mL), was added potassium carbonate (2.2 eq. amount) and the Schiff base **H(O,N)**(2 eq. amount). The resulting mixture was refluxed under N_2 for 24 h. After cooling, the resulting precipitate was filtrated, redissolved in dichloromethane and recrystallised by slow addition of ethanol. Recrystallisations were performed twice to yield to the pure desired complexes.

AZPtON. Yield: 77%, 710 mg. Mp: 128-128 ºC. IR (KBr) ν = 3054, 2927, 2871, 1613, 1582, 1503, 1200, 767, 691 cm^{-1}. ^{1}H NMR ($CDCl_3$, 500 MHz) δ = 8.07 (s, 1H), 7.9 (dd, $^3J_{HH}$ = 7.5 Hz, $^3J_{HH}$ = 1.5 Hz, 1H), 7.84 (dd, $^3J_{HH}$ = 8 Hz, $^3J_{HH}$ = 2 Hz, 2H), 7.56-7.52(m, 3H), 7.34(d, $^3J_{HH}$ = 8.4 Hz, 2H), 7.21(d, $^3J_{HH}$ = 8.1 Hz, 2H), 7.14 (d, $^3J_{HH}$ = 8.1 Hz, 1H), 6.9 (td, $^3J_{HH}$ = 7.2 Hz, $^3J_{HH}$ = 1 Hz, 1H), 6.7 (td, $^3J_{HH}$ = 8.1 Hz, $^3J_{HH}$ = 1.5 Hz, 1H), 6.3-6.2 (m, 2H), 5.54 (d with broad ^{195}Pt satellites, $^3J_{HH}$ = 7.8 Hz, $^3J_{PtH}$ = 39 Hz, 1H), 3.94 (t, $^3J_{HH}$ = 6.6 Hz, 2H), 2.71(t, $^3J_{HH}$ = 7.2 Hz, 2H), 1.8-1.6 (m, 4H), 1.5-1.3 (m, 12H), 0,92 (m, 6H) ppm. ^{13}C NMR ($CDCl_3$, 500 MHz) δ= 167.8, 166.2, 165.1, 162.1, 152.9, 150.5, 142.2, 142.1, 135.6, 133.7, 131.5, 129.6, 129.2, 128.9, 127.5, 125.8, 125.2, 123.5, 115.1, 108.3, 103.4, 68.1, 35.4,

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31.8, 31.7, 31.6, 29.1, 28.8, 25.8, 22.7, 22.6, 14.1, 14.0 ppm. Anal. calcd. for $C_{37}H_{43}N_3O_2Pt$ (756.30): C, 58.72; H, 5.73; N, 5.55 %; found: C, 58.91; H, 5.65; N, 5.32 %.

BEPtON. Yield: 87%, 805 mg. Mp: 181-182ºC; IR (KBr) ν = 3041, 2927, 2853, 1611, 1584, 1426, 1206, 837, 716 cm^{-1}. ^1H NMR ($CDCl_3$, 500 MHz) δ = 9.7 (d with broad ^{195}Pt satellites, $^3J_{HH}$ = 5.8 Hz, $^3J_{PtH}$ = 39 Hz, 1H), 8.2 (d, $^3J_{HH}$ = 8.1 Hz, 1H), 8.1 (s, 1H), 7.66 (d, $^3J_{HH}$ = 8.5 Hz, 1H), 7.55 (dd, $^3J_{HH}$ = 8.1 Hz, $^3J_{HH}$ = 5.7 Hz, 1H), 7.5-7.4 (m, 3H), 7.36 (d, $^3J_{HH}$ = 7.6 Hz, 1H), 7.2-7.1 (m, 3H), 6.95 (t, $^3J_{HH}$ = 8.5 Hz, 1H), 6.6 (d, $^3J_{HH}$ = 2.4 Hz, 1H), 6.26 (dd, $^3J_{HH}$ = 8.5 Hz, $^3J_{HH}$ = 2.1 Hz, 1H), 5.67 (d with broad ^{195}Pt satellites, $^3J_{HH}$ = 7.8 Hz, $^3J_{PtH}$ = 41 Hz, 1H), 4.06 (t, $^3J_{HH}$ = 6.3 Hz, 2H), 2,71 (t, $^3J_{HH}$ = 7.5 Hz, 2H), 1.9-1.7 (m, 4H), 1.6-1.4 (m, 12H), 0,93 (m, 6H) ppm; ^{13}C NMR ($CDCl_3$, 500 MHz) δ = 167.7, 165.8, 161.5, 157.1, 153.3, 145.4, 142.7, 141.8, 137.0, 135.8, 135.7, 133.2, 131.6, 129.6, 128.9, 128.0, 126.5, 125.6, 122.4, 120.9, 119.7, 116.3, 107.5, 104.0, 68.1, 35.5, 31.9, 31.8, 31.7, 29.3, 28.8, 25.8, 22.7, 22.6,14.1,14.0 ppm. Anal. calcd. for $C_{38}H_{42}N_2O_2Pt$ (753.29): C, 60.55; H, 5.62; N, 3.72 %; found: C, 60.78; H, 5.81; N, 3.53 %.

PYPtON. Yield: 86%, 820 mg. Mp: 194-195 ºC. IR (KBr) ν = 3026, 2928, 2855, 1611, 1586, 1196, 753, 728 cm^{-1}. ^1H NMR ($CDCl_3$, 500 MHz) δ = 9.6 (d with broad ^{195}Pt satellites, $^3J_{HH}$ = 5.8 Hz, $^3J_{PtH}$ = 43 Hz, 1H), 8,07 (s, 1H), 7.8 (td, $^3J_{HH}$ = 7.5 Hz, $^3J_{HH}$ = 1.2 Hz, 1H), 7.61 (d, $^3J_{HH}$ = 7.5 Hz, 1H), 7.43 (d, $^3J_{HH}$ = 8.1 Hz, 2H), 7.36 (d, $^3J_{HH}$ = 7.5 Hz, 1H), 7.3-7.1 (m, 4H), 6.86 (t, d, $^3J_{HH}$ = 7.2 Hz, 1H), 6.6-6.5 (m, 2H), 6.2 (dd, $^3J_{HH}$ = 8.2 Hz, d, $^3J_{HH}$ = 1.8 Hz, 1H), 5.7 (d with broad ^{195}Pt satellites, $^3J_{HH}$ = 7.8 Hz, $^3J_{PtH}$ = 41 Hz, 1H), 4.0 (t, $^3J_{HH}$ = 6.6 Hz, 2H), 2.6 (t, $^3J_{HH}$ = 7.2 Hz, 2H), 1.9-1.7 (m, 4H), 1.5-1.3 (m, 12H), 0.9 (m, 6H) ppm. ^{13}C NMR ($CDCl_3$, 500 MHz) δ = 167.9, 165.7, 161.9, 152.9, 146.5, 145.5, 141.7, 138.7, 135.7, 134.8, 128.7, 128.4, 125.5, 122.8, 122.5, 120.5, 118.0, 116.4, 111.9, 107.3, 103.9, 68.1, 35.4, 31.8, 31.62, 31.61, 29.2, 28.8, 25.8, 22.6, 22.6, 14.1, 14.0 ppm. Anal. calcd. for $C_{36}H_{42}N_2O_2Pt$ (729.29): C, 59.25; H, 5.80; N, 3.84 %; found: C, 59.02; H, 5.92; N, 3.92 %.

SI-3. Intrinsic photoconductivity of complexes BEMON

In order to check the nature of photoconductivity, asymmetric samples were prepared in which the compounds were sandwiched between one ITO and one Al electrode. When photoconductivity is extrinsic, due to the different properties of the electrodes, different photocurrents are usually measured for different polarities of the applied field [3,4]. In contrast, a measurement of the same photoconductivity for different field signs is taken as an indication of intrinsic photoconductivity or, in

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any case, as evidence that photoconductivity is a bulk property, which is what really matters in order to justify the model used to derive photogeneration efficiency.

Figures SI-1 and SI-2 show the photocurrents measured for compounds **BEPdON** and **BEPtON**, respectively, in asymmetric cells with one ITO and one Al electrode. It is evident that photoconductivity does not depend on the sign of the electric field.

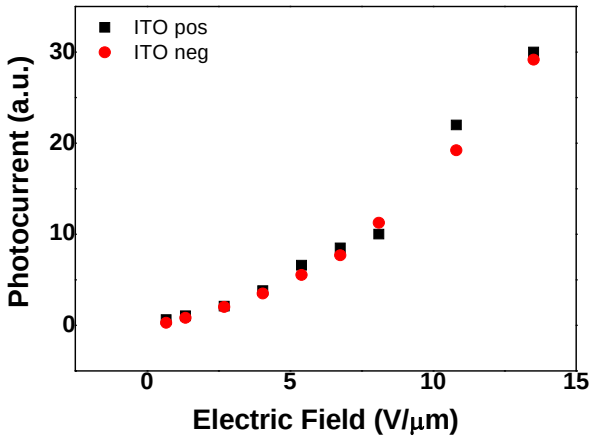

FIGURE SI-1. Electric field dependence of the photocurrent in an asymmetric cell of compound **BEPdON** with one ITO and one Al electrode.

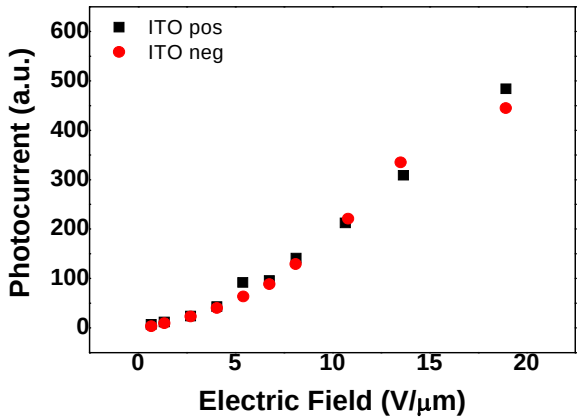

FIGURE SI-2. Electric field dependence of the photocurrent in an asymmetric cell of compound **BEPtON** with one ITO and one Al electrode.

SI-4. Absorption spectra

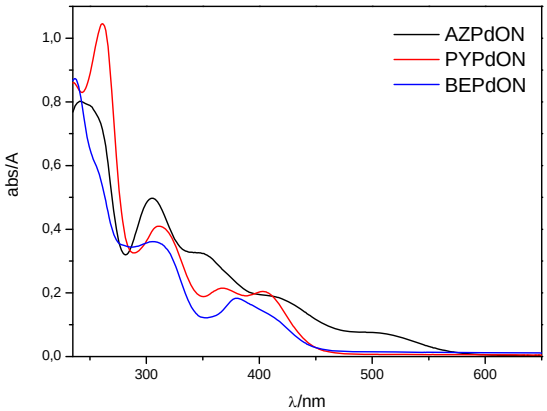

FIGURE SI-3. Absorption spectra of Pd-complexes recorded from dichloromethane deaerated solution at room temperature.

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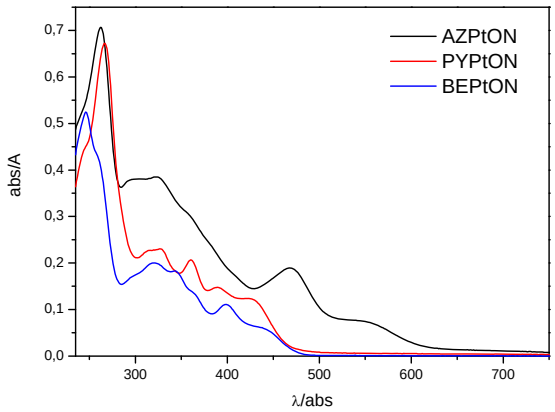

FIGURE SI-4. Absorption spectra of Pt-complexes recorded from dichloromethane deaerated solution at room temperature.

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SI-5. Ground state Cartesian coordinates obtained by DFT calculations. D95V/SDD/mPW1PW91 level of theory

AZPdON	Cartesian coordinates		
C	-3.440478	-1.869435	-0.234150
C	-2.047945	-1.595124	-0.124583
C	-1.117815	-2.673511	-0.309602
C	-1.626108	-3.978484	-0.585288
C	-2.974964	-4.229039	-0.706591
C	-3.887827	-3.151671	-0.528354
O	-1.671950	-0.367238	0.167570
Pd	0.199625	0.448643	-0.049139
N	1.004856	-1.430291	0.034474
C	0.286389	-2.531697	-0.131873
O	-5.217222	-3.496458	-0.667669
C	-6.222081	-2.466955	-0.505849
N	-0.533142	2.352583	0.041923
N	0.235485	3.319139	-0.338503
C	1.496400	2.885519	-0.743295
C	1.800386	1.490264	-0.650404
C	3.062293	1.109022	-1.136550
C	3.971823	2.059372	-1.634790
C	3.655452	3.429927	-1.675402
C	2.402013	3.847892	-1.230127
C	-1.840388	2.748799	0.472245
C	-2.463813	3.870394	-0.104471
C	-3.724040	4.270009	0.348783
C	-4.360118	3.563031	1.382888
C	-3.729459	2.447516	1.954080
C	-2.474442	2.029772	1.496559
C	2.394839	-1.629008	0.346883
C	2.947511	-0.983706	1.464609
C	4.289225	-1.183430	1.797214
C	5.119450	-2.023277	1.026837
C	4.554667	-2.655812	-0.093747
C	3.207335	-2.465157	-0.433928
C	6.569213	-2.225861	1.397629
H	0.837305	-3.473149	-0.081524
H	-0.919244	-4.795206	-0.707151
H	-3.366716	-5.213604	-0.926281
H	-4.113289	-1.033943	-0.089619
H	-6.092913	-1.670980	-1.247719
H	-6.188058	-2.038636	0.502265
H	2.319254	-0.325730	2.054118
H	4.700500	-0.677106	2.665648
H	5.172951	-3.296125	-0.715754
H	2.801655	-2.937732	-1.323123
H	7.105344	-1.271320	1.439152
H	6.663343	-2.693983	2.384147
H	3.363110	0.070257	-1.129608
H	4.940799	1.723158	-1.992310
H	4.372707	4.147961	-2.057059
H	2.098904	4.888737	-1.257918
H	-1.990739	1.159618	1.917639
H	-4.213907	1.899406	2.755100
H	-5.336331	3.877771	1.736721
H	-4.209109	5.129493	-0.101568

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H	-1.955539	4.410127	-0.894056
H	-7.176693	-2.966814	-0.662517
H	7.081809	-2.866343	0.675002

AZPtON Cartesian coordinates

C	3.53970	-1.82154	0.03820
C	2.13805	-1.58273	-0.00783
C	1.25226	-2.69424	-0.20063
C	1.81317	-3.99842	-0.35556
C	3.17234	-4.21569	-0.33710
C	4.04077	-3.10615	-0.13132
O	1.71023	-0.34631	0.15053
Pt	-0.19698	0.41132	-0.12221
N	-0.91790	-1.49061	-0.04275
C	-0.16124	-2.57926	-0.13324
O	5.38299	-3.42453	-0.11186
C	6.34474	-2.36590	0.11247
N	0.47404	2.31871	-0.00838
N	-0.39379	3.28483	-0.00874
C	-1.68386	2.84136	-0.28150
C	-1.87945	1.43575	-0.47580
C	-3.15801	1.06520	-0.93662
C	-4.17218	2.01726	-1.12457
C	-3.96061	3.38620	-0.86163
C	-2.69913	3.80474	-0.44555
C	1.82959	2.73111	0.21442
C	2.10844	3.73013	1.16161
C	3.42696	4.15894	1.34453
C	4.46218	3.60479	0.57452
C	4.17093	2.61441	-0.37607
C	2.85705	2.16679	-0.55444
C	-2.31676	-1.74967	0.19958
C	-3.06586	-2.53959	-0.68353
C	-4.41649	-2.80420	-0.41308
C	-5.04058	-2.29587	0.73889
C	-4.26861	-1.50600	1.61490
C	-2.92446	-1.23155	1.35323
C	-6.49265	-2.58296	1.03720
H	-0.69920	-3.52717	-0.09899
H	1.13912	-4.84005	-0.49129
H	3.60558	-5.19969	-0.46028
H	4.17596	-0.96285	0.20969
H	6.18628	-1.89055	1.08687
H	6.28927	-1.61023	-0.67928
H	-2.60647	-2.91777	-1.59158
H	-4.98953	-3.40653	-1.11152
H	-4.72764	-1.09826	2.51071
H	-2.33938	-0.61185	2.02304
H	-6.96499	-3.14432	0.22673
H	-6.59820	-3.17129	1.95597
H	-3.38301	0.02999	-1.15644
H	-5.14367	1.68668	-1.48060
H	-4.76228	4.10254	-1.00217
H	-2.46715	4.84894	-0.26726
H	2.61974	1.40004	-1.27894
H	4.96564	2.19359	-0.98313
H	5.48366	3.94345	0.71301
H	3.64608	4.92341	2.08227
H	1.29539	4.15518	1.73778

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H	7.31933	-2.85090	0.09190
H	-7.05975	-1.65650	1.17881

PYPdON Cartesian coordinates

C	-3.52261	4.23477	-2.82379
C	-3.99948	3.27786	-1.92528
C	-3.09225	2.54116	-1.14405
N	-1.74854	2.76779	-1.27627
C	-1.27820	3.69247	-2.14153
C	-2.13941	4.45093	-2.93514
C	-3.41604	1.53162	-0.14021
C	-4.73772	1.23941	0.24655
H	-5.57639	1.72518	-0.24348
H	-5.06234	3.09863	-1.82803
C	-4.97974	0.33626	1.28393
C	-3.88964	-0.25551	1.94257
C	-2.57294	0.02507	1.54546
C	-2.29381	0.90185	0.48061
Pd	-0.52745	1.55048	-0.20965
O	1.09319	2.64376	-0.89883
C	2.31014	2.64557	-0.39143
C	2.78491	1.62808	0.50485
C	4.12999	1.70158	0.97306
C	4.98048	2.72625	0.61727
C	4.50149	3.72868	-0.26887
C	3.20544	3.68623	-0.76967
C	2.02571	0.47652	0.86995
N	0.74770	0.20679	0.66075
C	0.32823	-1.12605	1.00328
C	0.59518	-1.67558	2.26691
C	0.19440	-2.98648	2.56355
C	-0.47453	-3.77581	1.61318
C	-0.73718	-3.20609	0.35083
C	-0.34703	-1.90065	0.04645
C	-0.90799	-5.18777	1.92748
O	5.42113	4.71294	-0.57735
C	5.02620	5.77432	-1.47722
H	-0.19969	3.79058	-2.16214
H	-1.73404	5.18538	-3.61937
H	-4.21769	4.80481	-3.43038
H	-5.99609	0.10921	1.58798
H	-4.06301	-0.93885	2.76880
H	-1.76514	-0.45401	2.08323
H	2.60856	-0.31302	1.34879
H	2.82368	4.43513	-1.45205
H	5.99829	2.79032	0.97912
H	4.48934	0.91930	1.63683
H	-0.56604	-1.46385	-0.92116
H	-1.25855	-3.79147	-0.40108
H	0.39694	-3.39251	3.55015
H	1.08301	-1.07289	3.02704
H	-0.66621	-5.46104	2.95812
H	-1.98846	-5.31028	1.79292
H	-0.41484	-5.90953	1.26626
H	5.90001	6.41786	-1.56802
H	4.75514	5.37631	-2.46184
H	4.18574	6.34620	-1.06746

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PYPtON	Cartesian coordinates		
C	-3.52261	4.23477	-2.82379
C	-3.99948	3.27786	-1.92528
C	-3.09225	2.54116	-1.14405
N	-1.74854	2.76779	-1.27627
C	-1.27820	3.69247	-2.14153
C	-2.13941	4.45093	-2.93514
C	-3.41604	1.53162	-0.14021
C	-4.73772	1.23941	0.24655
H	-5.57639	1.72518	-0.24348
H	-5.06234	3.09863	-1.82803
C	-4.97974	0.33626	1.28393
C	-3.88964	-0.25551	1.94257
C	-2.57294	0.02507	1.54546
C	-2.29381	0.90185	0.48061
Pd	-0.52745	1.55048	-0.20965
O	1.09319	2.64376	-0.89883
C	2.31014	2.64557	-0.39143
C	2.78491	1.62808	0.50485
C	4.12999	1.70158	0.97306
C	4.98048	2.72625	0.61727
C	4.50149	3.72868	-0.26887
C	3.20544	3.68623	-0.76967
C	2.02571	0.47652	0.86995
N	0.74770	0.20679	0.66075
C	0.32823	-1.12605	1.00328
C	0.59518	-1.67558	2.26691
C	0.19440	-2.98648	2.56355
C	-0.47453	-3.77581	1.61318
C	-0.73718	-3.20609	0.35083
C	-0.34703	-1.90065	0.04645
C	-0.90799	-5.18777	1.92748
O	5.42113	4.71294	-0.57735
C	5.02620	5.77432	-1.47722
H	-0.19969	3.79058	-2.16214
H	-1.73404	5.18538	-3.61937
H	-4.21769	4.80481	-3.43038
H	-5.99609	0.10921	1.58798
H	-4.06301	-0.93885	2.76880
H	-1.76514	-0.45401	2.08323
H	2.60856	-0.31302	1.34879
H	2.82368	4.43513	-1.45205
H	5.99829	2.79032	0.97912
H	4.48934	0.91930	1.63683
H	-0.56604	-1.46385	-0.92116
H	-1.25855	-3.79147	-0.40108
H	0.39694	-3.39251	3.55015
H	1.08301	-1.07289	3.02704
H	-0.66621	-5.46104	2.95812
H	-1.98846	-5.31028	1.79292
H	-0.41484	-5.90953	1.26626
H	5.90001	6.41786	-1.56802
H	4.75514	5.37631	-2.46184
H	4.18574	6.34620	-1.06746

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BEPdON Cartesian coordinates

C	0.21314	-1.36883	2.64933
C	0.19778	-0.96399	1.30610
C	-0.44317	-1.76977	0.35152
C	-1.04840	-2.96696	0.73988
C	-1.04018	-3.39167	2.08424
C	-0.40317	-2.57016	3.02934
N	0.84650	0.24992	0.88839
C	2.12714	0.34724	1.20621
C	3.08621	1.33688	0.83788
C	2.84856	2.34962	-0.15261
C	3.92118	3.21657	-0.50656
C	5.16388	3.09881	0.10488
C	5.40944	2.09897	1.08465
C	4.38439	1.24102	1.42091
O	1.69000	2.49845	-0.76363
Pd	-0.12007	1.68341	-0.19621
C	-2.03850	1.30250	0.30540
C	-2.94653	2.10214	-0.46096
C	-4.35869	2.06895	-0.31341
C	-4.90204	1.21154	0.67224
C	-4.03835	0.46012	1.46347
C	-2.63041	0.50273	1.28815
C	-5.16164	2.92067	-1.15834
C	-4.59742	3.77532	-2.07328
C	-3.16683	3.85819	-2.21349
C	-2.37967	3.01281	-1.39588
N	-1.01055	3.03503	-1.43278
C	-0.37458	3.86724	-2.26852
C	-1.09183	4.72975	-3.12300
C	-2.48476	4.72819	-3.09680
O	6.24587	3.91204	-0.17322
C	6.09065	4.96112	-1.15697
C	-1.69900	-4.68945	2.48705
H	0.70677	3.82794	-2.23188
H	-0.54443	5.38680	-3.78716
H	-3.04932	5.39115	-3.74470
H	-6.24176	2.87847	-1.05148
H	-5.22159	4.40905	-2.69555
H	-5.97693	1.15671	0.81455
H	-4.44528	-0.18419	2.23751
H	-2.02507	-0.11062	1.94278
H	2.53209	-0.47205	1.80397
H	3.71545	3.96611	-1.26023
H	6.39252	2.03510	1.53239
H	4.56330	0.46292	2.15859
H	-0.46813	-1.44100	-0.68115
H	-1.53937	-3.57966	-0.01066
H	-0.39373	-2.86383	4.07478
H	0.67485	-0.73327	3.39867
H	-1.67934	-4.82844	3.57123
H	-2.74503	-4.72179	2.16321
H	-1.19181	-5.54802	2.03170
H	7.05629	5.46260	-1.20120
H	5.84325	4.54610	-2.14078
H	5.31599	5.67451	-0.85316

BEPtON Cartesian coordinates

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C	1.87528	-1.49588	2.43991
C	1.25513	-1.28932	1.19972
C	0.54005	-2.33684	0.59933
C	0.45547	-3.57703	1.23615
C	1.07237	-3.80566	2.48305
C	1.77898	-2.74395	3.07276
N	1.36818	-0.02419	0.51745
C	2.61003	0.37036	0.27328
C	3.08092	1.47816	-0.48951
C	2.23976	2.29334	-1.31790
C	2.84066	3.31137	-2.10881
C	4.21361	3.52482	-2.06755
C	5.05760	2.72237	-1.25234
C	4.48692	1.72131	-0.49661
O	0.93188	2.12864	-1.39638
Pt	-0.26809	0.99728	-0.12156
C	-1.69257	0.24810	1.10008
C	-2.99952	0.72100	0.74537
C	-4.19336	0.37992	1.43352
C	-4.08806	-0.46300	2.56396
C	-2.82614	-0.89568	2.96345
C	-1.64982	-0.54836	2.25249
C	-5.44236	0.92569	0.95812
C	-5.49920	1.78314	-0.11313
C	-4.29725	2.17947	-0.80003
C	-3.07595	1.63000	-0.34393
N	-1.87127	1.96230	-0.91126
C	-1.83001	2.82717	-1.93799
C	-3.00788	3.40355	-2.45047
C	-4.24141	3.08393	-1.88565
O	4.86949	4.50107	-2.79180
C	4.09216	5.36927	-3.64921
C	0.97091	-5.15288	3.15762
H	-0.84373	3.04134	-2.32834
H	-2.93420	4.09458	-3.28076
H	-5.15541	3.52583	-2.26912
H	-6.35494	0.64744	1.47739
H	-6.44989	2.18456	-0.44991
H	-4.97709	-0.75001	3.11679
H	-2.73123	-1.52302	3.84516
H	-0.70802	-0.92156	2.63194
H	3.39427	-0.26996	0.67871
H	2.17988	3.90565	-2.72694
H	6.12236	2.91554	-1.25303
H	5.12307	1.09237	0.12077
H	0.04904	-2.15997	-0.35070
H	-0.10197	-4.37899	0.76100
H	2.25251	-2.88669	4.03947
H	2.40026	-0.67801	2.92356
H	1.42903	-5.13909	4.15012
H	-0.07378	-5.46120	3.27412
H	1.47427	-5.92844	2.56875
H	4.81228	6.04698	-4.10518
H	3.57767	4.79591	-4.42881
H	3.35960	5.94212	-3.06918

SI-6.X-Ray analyses and DFT calculations

Complexes **AZMON** and **PYMON** are characterized by the presence of two metallacycles, one being an N,O six-membered ring obtained by chelation of the Schiff base ligand to the metal ion and

the second one (a C,N five-membered ring) arising from the cyclometalation of one of the two C,N donor ligands, azobenzene and 2-phenylpyridine, respectively. In all cases, the metal center is found in a distorted square planar geometry and in an N,N *trans* configuration (Figure SI-5). Selected bond distances and angles are given in Table SI-1.

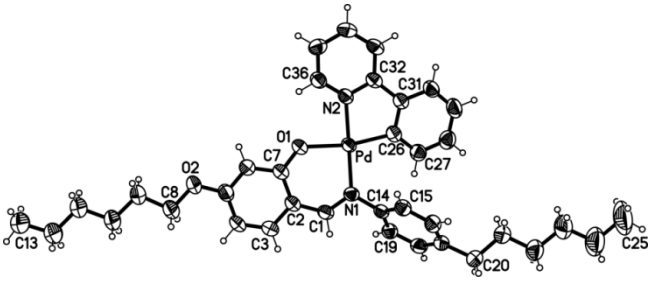

Figure SI-5. Perspective view of complex **PYPdON** with atomic numbering scheme (ellipsoids at the 50% level).

All complexes crystallize in the triclinic *P*-1 space group, with two molecules in the asymmetric unit only for the **AZPdON** and **AZPtON** derivatives. In both cases, one of the two molecules shows some disorder on the aliphatic chains of the Schiff base ligand, thus breaking the symmetry. Moreover, only in one of the two molecules of the asymmetric unit a severe distortion from the planarity of the N,O six-membered rings [M(1)-O(1)-C(7)-C(2)-C(1)] (puckering amplitude Q_t = 0.411(3) and Q_t = 0.360(3) Å in **AZPdON** and **AZPtON**, respectively) is observed. The N,O six-membered ring adopts an envelope conformation in M(1), with a slight deformation towards a boat one in C(2), as shown by the puckering angles ϕ_2 = 180.0(6)°, θ_2 = 114.6(4)° in **AZPdON** and ϕ_2 = 177.1(8)°, θ_2 = 113.2(6)° in **AZPtON**,respectively [5].In both **AZPdON** and **AZPtON**, in one of the two molecules of the asymmetric unit, the M(1) ion is located ~ 0.7 Å away from the best mean plane passing through the remaining five atoms. The dihedral angles between the mean planes passing through the almost planar five-membered MNCCC and the OCCCN rings are 22° in **AZPdON** and 18° in **AZPtON**. The second molecule of the asymmetric unit in both complexes is found to be more planar around the metal ion, with a puckering amplitude Q_t~0.07 Å for the N,O six-membered ring in both cases, and dihedral angles between the two metallacycles of 11° and 9° in **AZPdON** and **AZPtON**, respectively.

Table SI-1. Selected bond distances (Å) and angles (degrees) for complexes **AZMON** and **PYMON**

	AZPdON	**AZPtON**	**PYPdON**	**PYPtON**
M-N(1)	2.034(3) 2.034(3)	2.003(3) 1.999(4)	2.045(2)	2.020(4)
M-O(1)	2.041(3) 2.039(3)	2.030(3) 2.041(3)	2.063(2)	2.071(4)
M-N(2)	2.028(3) 2.027(3)	1.977(4) 1.979(4)	2.026(3)	2.015(5)

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M-C(26)	1.984(4) 1.975(4)	1.969(4) 1.974(5)	1.996(3)	2.001(5)
N(1)-M-O(1)	88.1(1) 90.6(1)	88.6(1) 89.6(1)	90.47(9)	90.1(2)
N(1)-M-N(2)	178.3(1) 170.4(2)	178.2(1) 171.9(2)	174.9(1)	175.7(2)
N(1)-M-C(26)	100.5(2) 101.1(2)	100.7(2) 101.6(2)	100.8(1)	101.4(2)
N(2)-M-C(26)	78.9(2) 78.7(2)	78.9(2) 78.6(2)	81.0(1)	80.8(2)
C(26)-M-O(1)	171.0(1) 168.4(2)	170.5(2) 168.8(2)	168.6(1)	168.4(2)
O(1)-M-N(2)	92.5(1) 90.0(1)	91.8(1) 90.5(2)	87.99(9)	87.9(2)

For **PYPdON** and **PYPtON**, the conformation of the N,O six-membered ring is found far from planarity, being also in these cases an envelope in M (parameters in **PYPdON**: Q_t = 0.200(2) Å, ϕ_2 = 176.7(9)° and θ_2 = 116.0(9)°; in **PYPtON**: Q_t = 0.188(4) Å, ϕ_2 = 0.7(18)° and θ_2 = 65.3(15)°) with a slight deviation to a boat one in C(2). In both cases, the metal ion is placed about 0.3 Å away from the mean plane passing through the OCCCN atoms, and the dihedral angles between this plane and the five-membered metalacycle are of about 9°.

An interesting feature arises when considering the degree of tilt (defined as the mean torsion angle around the C-N bond) of the rotationally free phenyl ring of the metal complexed Schiff base, which is a ligand common to all four derivatives (Table SI-2). In all cases, there is a strong tendency towards the orthogonality of this phenyl ring with respect to the mean plane passing through the cyclometalated ligand, giving the hydrogen atom in the *ortho* position with respect to the cyclometalated carbon atom of the CN ligand, the opportunity to point directly towards the top of the phenyl plane (Figure SI-6).

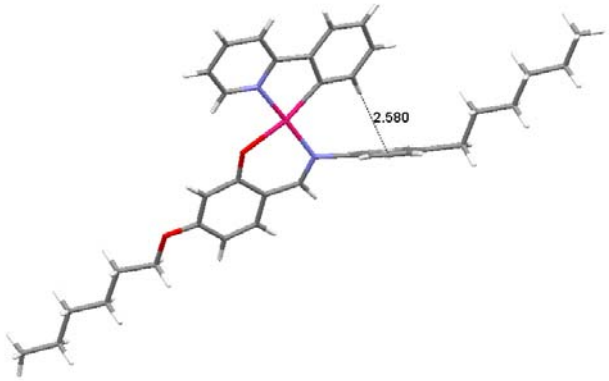


Figure SI-6. Perspective view of complex **PYPdON** showing the formation of intramolecular CH/π interactions.

The presence of a CH/π attractive intramolecular interaction between this hydrogen atom and the rotationally free phenyl ring is the structural feature characterizing this conformation. This interaction is characterized by very short H---phenyl plane distances and all geometrical parameters are indicative of its presence (Table SI-2).[6]

Despite of the difference between the C,N donor ligands, azobenzene and 2-phenylpyridine, all four complexes are characterized by a crystal packing dominated by the segregation of the aliphatic chains on the complexed Schiff base, with the repetition of polar (metal containing) and apolar sub-layers (Figure SI-7).

Table SI-2. Selected structural parameters concerning CH/π intramolecular interactions for complexes **AZMON** and **PYMON**

Complex	τ (C-N-C-Cph)[a] (°)	H---G(Ph) (Å)[b]	H---Ph (Å) (plane)[c]	γ (°) angle[d]
AZPdON	54.2(4)	2.68	2.50	21.1
	67.0(7)	2.65	2.50	19.5
AZPtON	53.6(6)	2.66	2.50	20.4
	67.5(6)	2.58	2.44	18.5
PYPdON	59.4(4)	2.58	2.41	20.6
PYPtON	60.8(7)	2.56	2.40	20.3

[a] τ is defined as (τ1 + τ2 + 180)/2, where τ1 and τ2 are C(1)-N(1)-C(14)-C(15) and C(1)-N(1)-C(14)-C(19), respectively; [b] *H*---G(Ph): separation between the hydrogen atom (H(27a)) and the centroid of the phenyl ring in the reported CH/πintramolecular interactions; [c] *H*---Ph(plane): distance between the hydrogen atom and the phenyl plane in the reported CH/πintramolecular interactions; [d] γ: the angle between the *H*---G(Ph) vector and the normal to the phenyl ring.

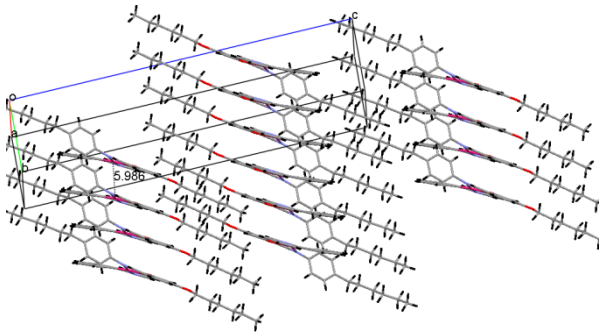
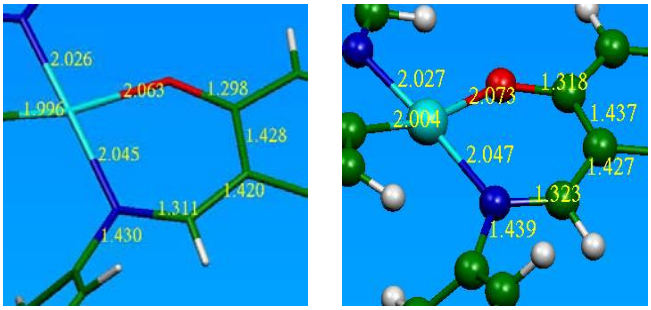


Figure SI-7. Crystal packing view of complex **PYPdON**.

DFT results and X-Ray data are in good agreement. Figure SI-8 shows some of the most relevant geometrical features around the metal atom in the case of complex **PYPdON**.



a) b)

Figure SI-8. Comparison between the X-Ray (a) and DFT (b) results for bond distances (Å) near the co-ordination sphere in the case of **PYPdON**.

Calculated cartesian coordinates for the other compounds are reported in the Supporting Information. The largest deviation between computational and experimental results can be observed for the O-phenyl bond distance within the six-membered palladacycle, being 1.298(3) Å and 1.318 Å in the case of X-rays and DFT, respectively (similar deviations are obtained by using the B98 and PBE1PBE xc functionals). Even though shorter alkyl chains were used, in the whole set of molecules computations reproduce well both the deviation from planarity in the coordination sphere of the square-planar complexes and the orientation of the phenyl ring of the Schiff's base. The bond angles around the Pd centres are fairly well reproduced (see Table SI-3). Within the five-membered MNCCC cycle, the torsional angle between the phenyl and the pyridine moieties is 2.8(4)° and 3.2°, in the case of X-ray and D95V(d)/SDD/mPW1PW91 DFT computations, respectively. When compared with diffraction data, the deviation from coplanarity between the two metallacyles is slightly more pronounced in the structure of **PYPdON** obtained from the DFT calculation, with a dihedral angle of about 16°. These

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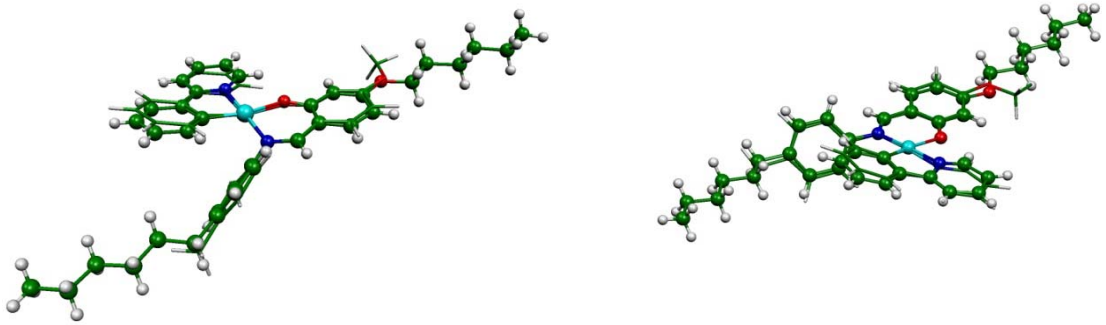
findings suggest that the lack of planarity is mainly due to intramolecular rather than intermolecular interactions. Indeed, even in the isolated molecule the rotationally free phenyl ring of the Schiff base shows a tilt angle of 52.1° in the case of **PYPdON**, and a comparable C-H/π interaction, characterized by structural parameters of 2.62 Å, 2.39 Å and 24.2° (see Table SI-2 for experimental data).

Comparable deviation between X-Ray and DFT results have been found in the case of **AZPdON,AZPtON** and **PYPtON**.

Table SI-3. Comparison between X-Ray and DFT (obtained by using different xc funtionals) values of bond angle (degrees) around the metal atom in **PYPdON**

Bond angle	X-Ray	mPW1PW91	B98	PBE1PBE
N(py)-Pd-C(ph)	81.0(1)	81.04	80.90	80.91
C(ph)-Pd-N(Schiff)	100.8(1)	100.95	101.01	100.11
N(Schiff)-Pd-O	90.47(9)	90.04	89.93	90.20
O-Pd-N(py)	87.99(9)	88.84	88.96	89.09



PYPdON **PYPtON**

FIGURE SI-9. Overlap between X-Ray and computed structures at D95V/SDD/mPW1PW91 level of theory. (ball and stick) and (stick) models, respectively.

SI-7. CV of AZPtON

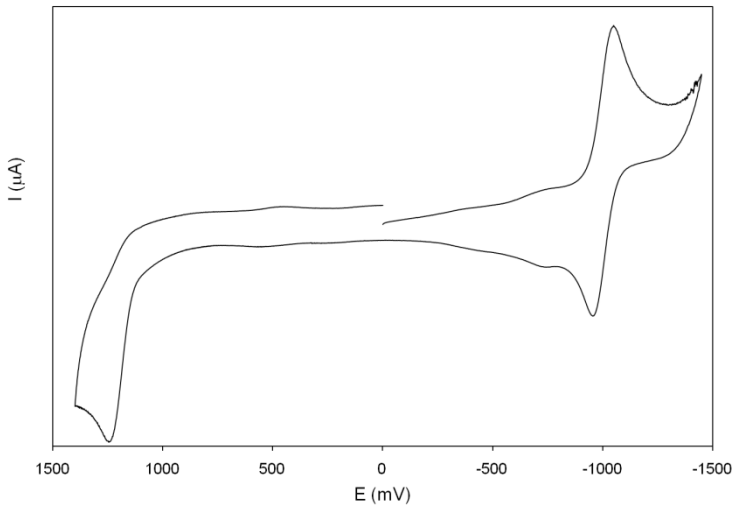


FIGURE SI-10. CV of **AZPtON**, 10^{-3}M in CH_2Cl_2 working electrode Pt button. Supporting electrolyte $N(C_4N_9\text{-}n)_4BF_4$0.15 M. Scan rate 200 mV sec^{-1}.

SI-8. Comparison between CV and DFT results

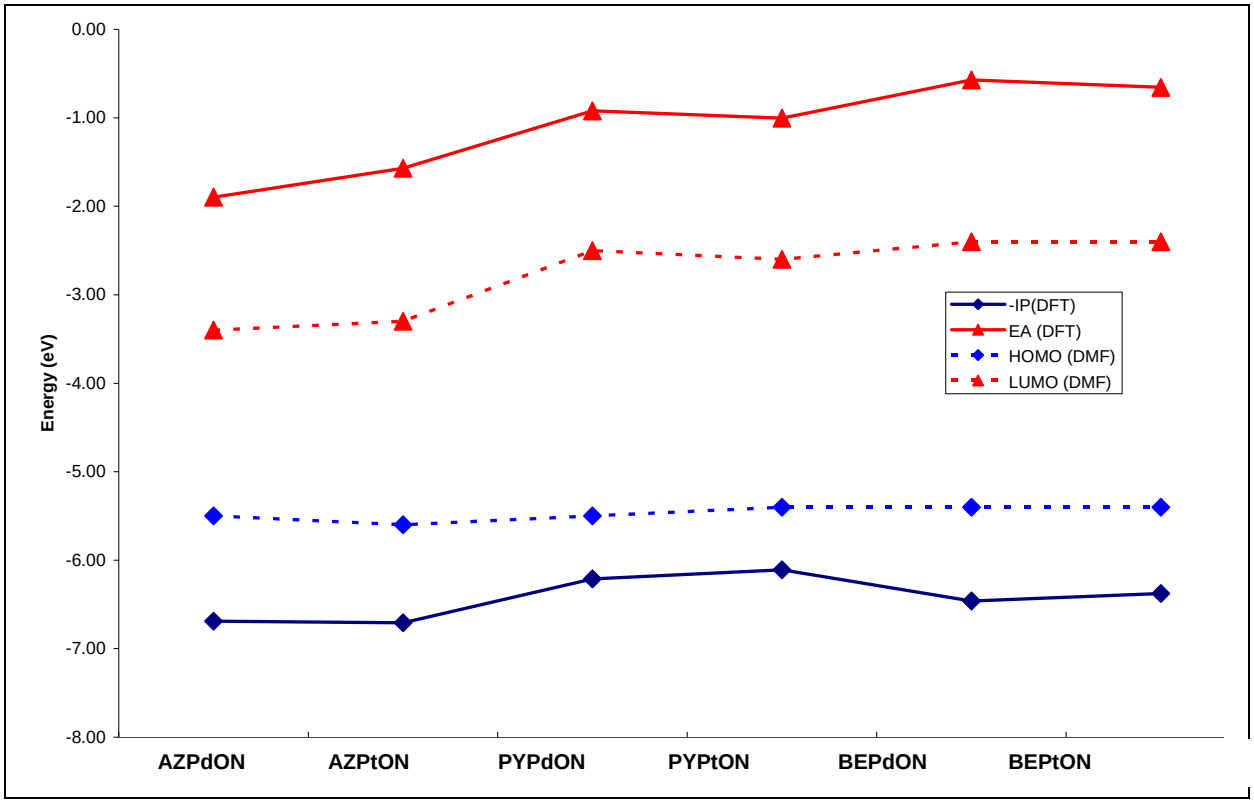


FIGURE SI-11. Comparison between computed (full lines) and CV "HOMO" and "LUMO" energies. Lines joining points are introduced only for comparison purposes.

HOMO and LUMO energies obtained by DFT at the SDD/D95V(d,p)/mPW1PW91 level of theory, without taking into account solvent effects, appear to be less and more bound, respectively, when compared with the experimental CV energies, as illustrated in Figure SI-11.

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Both experimental and computational results show the same trend in the oxidation potentials of the different compounds, especially considering that most of the CV results involve irreversible processes: **AZPdON**~ **AZPtON**>**BEPdON**~ **BEPtON**>**PYPdON**~ **PYPtON**. In addition, the reduction potentials of **AZPdON** and **AZPtON** are quite different from those of the other complexes.

SI-9. Gaussian functions used in the UV-Vis decomposition spectrum

	AZPdON			**AZPtON**		
	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})
1	42259.00	11694.79	2603.20	43467.28	6193.561	43467.28
2	41060.64	850.06	775.40	40958.90	3177.117	40958.9
3	39939.67	1650.57	836.32	39498.79	3022.273	39498.79
4	38193.56	8300.17	1537.11	37733.44	8715.428	37733.44
5	35495.79	2727.47	1340.46	34830.60	3382.547	34830.6
6	33525.76	5428.16	1277.14	33884.43	1339.58	33884.43
7	32455.91	1229.07	920.16	32517.71	1056.625	32517.71
8	31388.01	4688.45	1249.18	32254.94	2030.817	32254.94
9	29767.48	1716.15	1030.15	31160.58	2034.084	31160.58
10	28343.95	3252.54	1345.88	29400.51	4063.692	29400.51
11	26566.99	308.40	684.83	27530.59	2408.901	27530.59
12	25706.91	2553.60	2356.29	26087.83	2155.867	26087.83
13	23443.25	543.87	1259.82	24352.11	2229.957	24352.11
14	22376.70	573.67	2467.31	22579.04	1237.467	22579.04
15	21083.10	411.13	2332.52	21190.22	2561.268	21190.22
16	19385.01	536.53	1179.77	19495.18	734.7294	19495.18
17	15675.01	27.33	1327.76	18026.79	858.7694	18026.79
18	14073.88	13.89	868.58	16847.60	25.82474	16847.6
19	-------	------	-------	15391.67	188.4755	15391.67

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	PYPdON			PYPtON		
	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})
1	42840.51	13616.62	2811.65	41944.27	12397.50	2462.91
2	38555.49	11245.32	1822.96	40960.65	1023.41	807.18
3	37595.94	2978.96	1007.67	38518.06	12598.71	1627.63
4	35719.03	3711.71	2241.01	38285.43	2188.99	774.50
5	33973.42	1817.84	1052.42	37117.39	9541.17	933.39
6	32412.64	4338.12	1066.96	36709.58	436.52	467.80
7	31190.61	1455.79	888.05	35530.73	7990.59	1318.34
8	30464.51	2855.10	1207.96	34959.22	976.26	1566.25
9	28048.84	2210.36	2212.65	33597.33	627.27	747.41
10	27171.21	1168.95	1068.81	31790.09	7348.18	1987.98
11	25640.45	1108.46	1046.88	30052.67	2594.30	794.46
12	24493.44	1958.55	912.24	28974.59	2126.61	609.64
13	23429.85	807.62	912.99	27755.64	5344.10	803.18
14	22018.42	65.67	824.04	25734.22	3974.11	1194.04
15	20380.00	109.34	6132.63	24747.25	855.30	3007.97
16	------	------	-------	24402.30	368.77	614.75
17	------	------	-------	23260.55	2994.92	1013.17
18	------	------	-------	17001.64	169.67	4319.94

	BEPdON			BEPtON		
	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})	ν_{max} (cm^{-1})	ε_{max} (arb.u.)	$\omega/2$ (cm^{-1})
1	42241.22	29131.98	2706.98	41960.93	15043.19	2220.30
2	39541.73	863.06	789.79	40326.11	5181.88	930.93

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3	38462.56	7479.18	1214.61	39014.20	2672.39	951.81
4	36263.87	8503.59	1821.21	37945.14	9688.50	1324.92
5	33582.87	7573.69	1794.92	35554.72	3606.88	1533.30
6	31943.78	5556.52	1439.85	33625.04	3165.84	1243.87
7	30793.72	3819.88	1071.91	31777.10	524.66	1968.69
8	29225.94	2995.53	1240.77	31330.81	5534.62	1490.59
9	27545.27	2807.24	949.14	30101.94	1536.15	801.76
10	26408.80	3946.89	714.87	28822.23	4434.36	843.20
11	25466.01	1822.15	667.69	27339.41	3677.51	804.49
12	24469.93	3856.61	1156.69	26255.73	1214.91	-568.77
13	22751.06	579.82	1154.52	25209.81	2995.84	746.11
14	21394.69	55.58	569.05	24098.09	1603.67	874.47
15	20436.84	175.86	1193.44	22616.05	1696.76	977.53
16	18816.69	334.48	2493.15	19720.00	28.83	948.49
17	14338.45	298.82	3111.04	17980.00	28.09	1378.61
18	------	--------	---------	14970.00	12.87	1358.24

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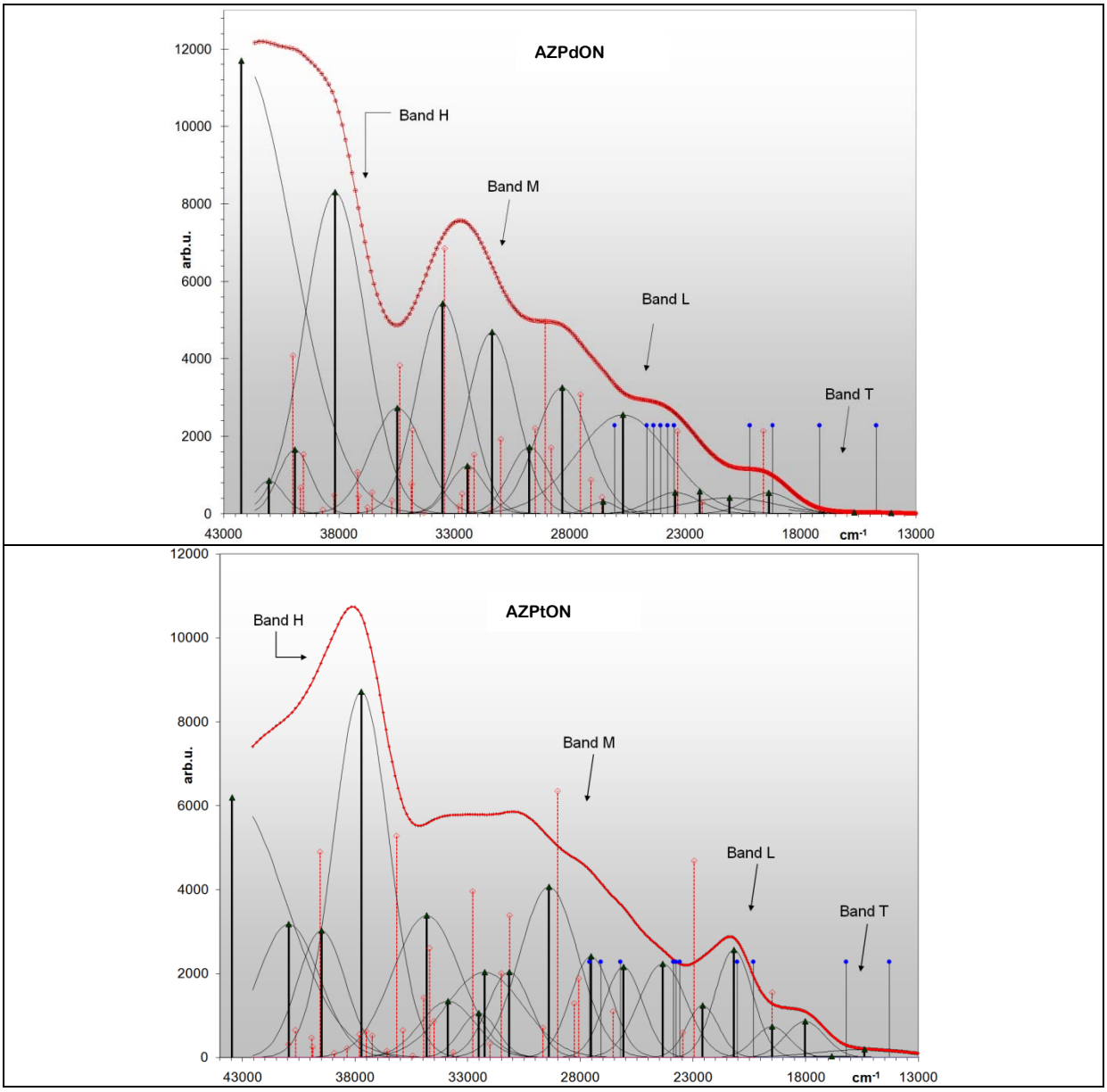
SI-10. Experimental (red line and hollow dots) and decomposed UV-Vis spectra (black line with crosses) as sum of Gaussian functions (black vertical arrows: position indicates wavenumber and height intensity); DFT computed transitions (red dashed line with hollow rhombus); computed triplet transitions (blue lines with blue dot)



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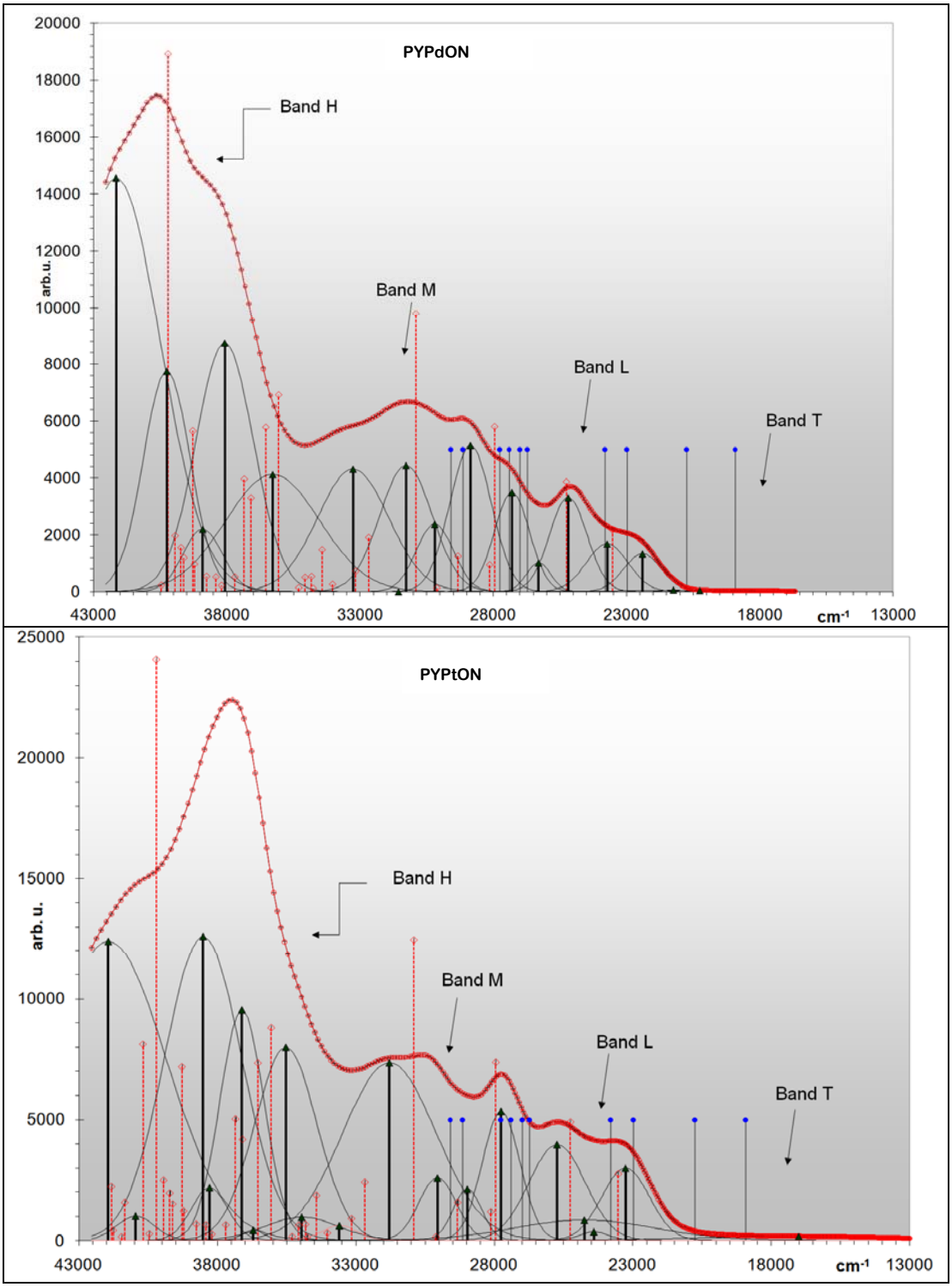
S-11.



Computational characterization of the excited states: composition in terms of monoelectronic excitation

AZPdON: D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 2.3853 eV 519.78 nm f=0.0623
119 ->121 0.16801
120 ->121 0.65603

Excited State 2: Singlet 2.7478 eV 451.21 nm f=0.0051

115 ->121 0.12224
117 ->121 0.45821
118 ->121 0.46021
119 ->121 0.14511

Excited State 3: Singlet 2.8472 eV 435.47 nm f=0.0675
112 ->121 -0.11609
116 ->121 -0.12258
118 ->121 -0.16796
119 ->121 0.59010
120 ->121 -0.18213

Excited State 4: Singlet 3.2501 eV 381.47 nm f=0.0285
115 ->121 0.14486
117 ->121 0.21448
118 ->121 -0.21249
120 ->122 0.54929
120 ->123 -0.13435

Excited State 5: Singlet 3.2931 eV 376.50 nm f=0.0420
109 ->121 0.13756
113 ->121 0.21491
115 ->121 0.37538
116 ->121 0.34255
118 ->121 -0.17411
120 ->122 -0.17733
120 ->123 0.17014

Excited State 6: Singlet 3.4003 eV 364.63 nm f=0.0592
116 ->121 0.42362
117 ->121 -0.30165
118 ->121 0.33171
119 ->121 0.17938
120 ->122 0.18508

Excited State 7: Singlet 3.5356 eV 350.67 nm f=0.0111
109 ->121 -0.10302
113 ->121 -0.10941
115 ->121 -0.20292
116 ->123 -0.10800
119 ->123 0.17163
120 ->122 0.17332
120 ->123 0.49660

Excited State 8: Singlet 3.5684 eV 347.45 nm f=0.2004
108 ->121 0.15065
109 ->121 -0.19017
112 ->121 0.13064
113 ->121 -0.18542
114 ->121 -0.21923
115 ->121 -0.13161
116 ->121 0.27876
117 ->121 0.29163
118 ->121 -0.13870
120 ->122 -0.14055
120 ->123 -0.19593

Excited State 9: Singlet 3.6657 eV 338.22 nm f=0.0613
109 ->121 0.13824
111 ->121 -0.12488
113 ->121 0.10414
114 ->121 0.44930

115 ->121 -0.34922
116 ->121 0.21713

Excited State 10: Singlet 3.8194 eV 324.62 nm f=0.0641
112 ->121 -0.11327
115 ->123 0.10109
117 ->122 -0.17593
117 ->123 0.37895
118 ->122 -0.17370
118 ->123 0.31392
119 ->122 -0.13737
120 ->123 -0.10591

Excited State 11: Singlet 3.8807 eV 319.49 nm f=0.0167
107 ->121 -0.10966
109 ->121 0.12393
110 ->121 0.22943
111 ->121 0.22766
112 ->123 -0.10275
113 ->121 0.34340
114 ->121 -0.14400
115 ->121 -0.23516
119 ->122 -0.16194
119 ->123 0.23799
120 ->123 -0.14113

Excited State 12: Singlet 3.9522 eV 313.71 nm f=0.0455
108 ->121 -0.11986
109 ->121 -0.11591
110 ->121 -0.12685
111 ->121 0.21660
112 ->121 0.48952
113 ->121 0.12989
114 ->121 0.17206
117 ->122 -0.10980
118 ->122 -0.15676
119 ->122 -0.12261
119 ->123 -0.10786

Excited State 13: Singlet 3.9645 eV 312.73 nm f=0.0284
109 ->121 -0.13725
112 ->123 0.11150
113 ->121 0.39425
114 ->121 -0.16456
115 ->121 -0.11511
118 ->123 0.11813
119 ->122 0.31382
119 ->123 -0.24274
120 ->123 0.10038

Excited State 14: Singlet 4.0241 eV 308.11 nm f=0.0039
109 ->121 -0.12675
114 ->121 0.11387
117 ->122 0.34152
117 ->123 0.16180
118 ->122 0.49212
118 ->123 0.12417
119 ->122 -0.11875

Excited State 15: Singlet 4.0636 eV 305.11 nm f=0.0061
108 ->121 -0.27082
109 ->121 0.34796

110 ->121	0.15587	
112 ->121	0.11851	
113 ->121	-0.15084	
114 ->121	-0.25229	
115 ->121	-0.13886	
118 ->122	0.10084	
118 ->123	0.11333	
119 ->123	-0.22961	

Excited State 16: Singlet 4.1082 eV 301.80 nm f=0.2446

112 ->121	0.18958	
113 ->121	-0.14268	
119 ->122	0.49954	
119 ->123	0.20112	

Excited State 17: Singlet 4.2208 eV 293.75 nm f=0.0040

107 ->121	-0.11978	
108 ->121	0.25464	
110 ->121	0.29673	
111 ->121	0.36990	
112 ->121	-0.14641	
113 ->121	-0.14924	
114 ->121	0.23620	
119 ->123	-0.18502	

Excited State 18: Singlet 4.2711 eV 290.29 nm f=0.0215

113 ->122	0.13696	
114 ->122	-0.13682	
115 ->122	0.34826	
116 ->122	0.50325	

Excited State 19: Singlet 4.3468 eV 285.23 nm f=0.2147

111 ->121	-0.11358	
115 ->122	0.17396	
116 ->122	-0.14164	
117 ->122	0.45135	
118 ->122	-0.33680	
120 ->129	0.10121	

Excited State 20: Singlet 4.3625 eV 284.21 nm f=0.0075

107 ->121	0.19060	
107 ->123	-0.16830	
108 ->121	-0.18332	
108 ->123	0.14446	
110 ->121	-0.15459	
110 ->123	0.12865	
111 ->121	0.31725	
112 ->121	-0.22684	
113 ->123	0.11566	
115 ->122	0.12115	
116 ->123	0.19323	
117 ->122	0.14155	
118 ->122	-0.13942	

Excited State 21: Singlet 4.3895 eV 282.46 nm f=0.0122

107 ->123	0.19876	
108 ->121	-0.18497	
108 ->123	-0.15110	
110 ->121	-0.25786	
110 ->123	-0.13979	
111 ->121	0.28799	
112 ->121	-0.17779	

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113 ->123 -0.11086
114 ->123 0.10350
115 ->122 -0.13773
115 ->123 -0.10201
116 ->123 -0.22828

Excited State 22: Singlet 4.5342 eV 273.44 nm f=0.0077
120 ->124 0.67413

Excited State 23: Singlet 4.5707 eV 271.26 nm f=0.0015
107 ->121 0.59271
108 ->121 0.10997
110 ->121 0.20083

Excited State 24: Singlet 4.6434 eV 267.01 nm f=0.0253
108 ->121 0.12392
111 ->123 0.10484
113 ->122 -0.10197
114 ->122 0.21622
115 ->122 -0.33421
116 ->122 0.35577
116 ->123 -0.13918
117 ->122 0.21251

Excited State 25: Singlet 4.6614 eV 265.98 nm f=0.0030
108 ->121 0.36688
109 ->121 0.37553
110 ->121 -0.30953
116 ->122 -0.10195

Excited State 26: Singlet 4.7130 eV 263.07 nm f=0.0046
110 ->123 0.15725
111 ->122 -0.10547
111 ->123 0.15485
114 ->122 0.23341
114 ->123 -0.12631
115 ->122 0.33189
116 ->122 -0.17923
116 ->123 -0.27121
120 ->123 -0.17200
120 ->127 0.13769

Excited State 27: Singlet 4.7825 eV 259.24 nm f=0.0135
110 ->123 -0.11624
111 ->122 -0.10126
111 ->123 -0.12644
114 ->122 0.45082
115 ->122 0.12512
116 ->123 0.19395
117 ->123 -0.14929
118 ->123 0.26826
120 ->123 0.10606

Excited State 28: Singlet 4.8905 eV 253.52 nm f=0.0109
120 ->125 0.68456

Excited State 29: Singlet 4.9298 eV 251.50 nm f=0.0798
112 ->122 -0.14248
114 ->122 0.12316
117 ->123 0.30155
118 ->123 -0.34015
120 ->126 0.38838

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120 ->127 -0.13136

Excited State 30: Singlet 4.9454 eV 250.71 nm f=0.0456
110 ->123 0.10494
114 ->122 -0.13624
116 ->123 -0.13160
117 ->123 -0.20976
118 ->123 0.25346
120 ->126 0.50224

Excited State 31: Singlet 4.9758 eV 249.17 nm f=0.0040
112 ->122 0.40902
113 ->122 -0.15300
118 ->123 -0.12985
119 ->124 0.13749
120 ->126 0.16675
120 ->127 0.38553

Excited State 32: Singlet 5.0184 eV 247.06 nm f=0.0145
111 ->122 0.35614
112 ->122 -0.18514
113 ->122 -0.22682
114 ->124 0.10791
118 ->124 -0.14121
119 ->124 -0.29265
120 ->124 -0.10558
120 ->127 0.31175

Excited State 33: Singlet 5.0711 eV 244.49 nm f=0.0080
108 ->122 0.11440
111 ->122 -0.12368
112 ->122 -0.24083
112 ->123 0.10420
113 ->122 0.34016
116 ->123 0.20040
119 ->123 0.11052
120 ->127 0.35592
120 ->129 0.10137

Excited State 34: Singlet 5.1725 eV 239.70 nm f=0.0510
108 ->123 -0.10690
111 ->122 -0.15664
112 ->122 -0.13242
112 ->123 0.17707
113 ->122 -0.45351
114 ->122 -0.18266
115 ->123 -0.11698
116 ->123 0.18906
119 ->123 0.18488
119 ->124 0.13304
120 ->128 0.11531

Excited State 35: Singlet 5.1825 eV 239.24 nm f=0.0817
111 ->122 -0.11797
115 ->123 -0.16700
119 ->123 0.15097
119 ->124 -0.11552
120 ->128 -0.54539
120 ->129 -0.14284

Excited State 36: Singlet 5.1889 eV 238.94 nm f=0.0499
112 ->122 0.28083

113 ->122 0.11865
113 ->123 -0.12205
115 ->123 -0.10924
116 ->123 0.16876
119 ->123 0.13615
119 ->124 -0.41339
120 ->127 -0.11155
120 ->128 0.27202

Excited State 37: Singlet 5.2367 eV 236.76 nm f=0.0671
111 ->122 0.42816
112 ->122 0.10642
112 ->123 0.18249
114 ->122 0.18952
116 ->123 0.10731
119 ->123 0.15935
119 ->124 0.29654

Excited State 38: Singlet 5.2480 eV 236.25 nm f=0.1941
115 ->123 0.17791
120 ->127 0.11018
120 ->128 -0.19970
120 ->129 0.53554

Excited State 39: Singlet 5.3173 eV 233.17 nm f=0.0002
105 ->121 0.60552
106 ->121 -0.19280
119 ->125 0.13044

Excited State 40: Singlet 5.3210 eV 233.01 nm f=0.0369
110 ->122 0.18581
115 ->123 0.14498
117 ->124 0.14451
118 ->124 0.36708
119 ->124 -0.18622
120 ->130 -0.40787

Excited State 41: Singlet 5.3320 eV 232.53 nm f=0.0831
111 ->122 0.14698
115 ->123 -0.10357
117 ->124 0.15712
118 ->124 0.38409
120 ->130 0.45615

AZPtON:D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 2.3648 eV 524.30 nm f=0.0496
119 ->121 0.28722
120 ->121 0.60018
Excited State 2: Singlet 2.8203 eV 439.61 nm f=0.1287
117 ->121 -0.11200
119 ->121 0.57780
120 ->121 -0.30125

Excited State 3: Singlet 2.8735 eV 431.47 nm f=0.0048
116 ->121 0.39719
117 ->121 0.23302
118 ->121 0.50473

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Excited State 4: Singlet 3.2133 eV 385.85 nm f=0.0470
116 ->121 0.10112
120 ->122 0.65010

Excited State 5: Singlet 3.4097 eV 363.62 nm f=0.0662
108 ->121 0.12948
111 ->121 0.11843
112 ->121 0.10399
113 ->121 -0.29725
115 ->121 0.30618
116 ->121 -0.13993
117 ->121 0.43314
118 ->121 -0.14311

Excited State 6: Singlet 3.4995 eV 354.30 nm f=0.0612
116 ->121 0.51078
118 ->121 -0.39896
119 ->122 -0.14401

Excited State 7: Singlet 3.6285 eV 341.69 nm f=0.1121
108 ->121 -0.30073
113 ->121 0.31035
114 ->121 -0.31390
115 ->121 -0.12589
117 ->121 0.33085
118 ->121 -0.10811

Excited State 8: Singlet 3.6815 eV 336.78 nm f=0.0784
108 ->121 0.14963
111 ->121 -0.15041
113 ->121 0.10778
114 ->121 0.39269
115 ->121 -0.37336
117 ->121 0.26108
118 ->121 -0.11926
119 ->122 0.12110

Excited State 9: Singlet 3.8173 eV 324.80 nm f=0.1374
112 ->121 -0.11387
115 ->121 0.13143
118 ->122 -0.16722
119 ->122 0.60469

Excited State 10: Singlet 3.8899 eV 318.73 nm f=0.0028
109 ->121 -0.11738
110 ->121 -0.13552
111 ->121 -0.19931
112 ->121 -0.16447
113 ->121 0.36740
114 ->121 0.15167
115 ->121 0.43936

Excited State 11: Singlet 3.9310 eV 315.40 nm f=0.0581
116 ->122 0.36514
117 ->122 0.22074
118 ->122 0.50877
119 ->122 0.12183

Excited State 12: Singlet 4.0025 eV 309.77 nm f=0.1056
109 ->121 -0.15536
110 ->121 -0.13840

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112 ->121	0.58912			
113 ->121	0.16931			
119 ->121	0.10619			
119 ->122	0.10930			
Excited State 13:	Singlet	4.1389 eV	299.56 nm	f=0.0122
107 ->121	-0.12233			
108 ->121	0.51099			
110 ->121	0.11992			
112 ->121	-0.10779			
113 ->121	0.21558			
114 ->121	-0.30130			
Excited State 14:	Singlet	4.2058 eV	294.79 nm	f=0.0096
119 ->124	0.12237			
120 ->123	-0.19428			
120 ->124	0.55546			
120 ->130	-0.21079			
Excited State 15:	Singlet	4.2485 eV	291.83 nm	f=0.0068
109 ->121	0.17561			
110 ->121	0.20608			
111 ->121	0.32628			
113 ->121	0.14987			
114 ->121	0.28935			
115 ->122	-0.11955			
116 ->122	0.31596			
117 ->122	-0.16506			
118 ->122	-0.11033			
Excited State 16:	Singlet	4.2708 eV	290.31 nm	f=0.0012
109 ->121	0.11670			
110 ->121	0.16323			
111 ->121	0.27206			
113 ->121	0.15124			
113 ->122	-0.15414			
114 ->121	0.13245			
115 ->122	0.22411			
116 ->122	-0.26800			
117 ->122	0.38117			
Excited State 17:	Singlet	4.3317 eV	286.23 nm	f=0.2601
113 ->122	-0.11842			
115 ->122	0.22218			
116 ->122	0.37444			
117 ->122	0.25293			
118 ->122	-0.36171			
Excited State 18:	Singlet	4.4520 eV	278.49 nm	f=0.0007
107 ->121	0.17224			
109 ->121	-0.20838			
110 ->121	-0.38532			
111 ->121	0.46202			
112 ->121	-0.17686			
Excited State 19:	Singlet	4.5068 eV	275.11 nm	f=0.0088
120 ->123	0.64354			
120 ->124	0.19613			
Excited State 20:	Singlet	4.5529 eV	272.32 nm	f=0.0559
111 ->122	-0.11758			
112 ->122	-0.13862			
113 ->122	0.24786			

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114 ->122	0.27642			
115 ->122	-0.33492			
117 ->122	0.36228			
118 ->122	-0.11055			
120 ->123	-0.11484			
Excited State 21:	Singlet	4.6341 eV	267.55 nm	f=0.0140
107 ->121	0.34510			
110 ->121	0.18663			
114 ->122	-0.30912			
115 ->122	-0.26132			
117 ->122	0.16259			
119 ->124	-0.26046			
120 ->124	0.12881			
Excited State 22:	Singlet	4.6804 eV	264.90 nm	f=0.0040
107 ->121	0.48269			
110 ->121	0.11833			
114 ->122	0.27940			
119 ->123	-0.11487			
119 ->124	0.19060			
Excited State 23:	Singlet	4.6908 eV	264.31 nm	f=0.0386
109 ->121	0.43171			
110 ->121	-0.22045			
114 ->122	0.14041			
116 ->124	-0.11061			
118 ->124	-0.12552			
119 ->123	0.11424			
119 ->124	-0.22463			
119 ->127	0.11082			
120 ->124	0.12745			
Excited State 24:	Singlet	4.7149 eV	262.96 nm	f=0.0063
109 ->121	0.27200			
110 ->121	-0.22505			
114 ->122	-0.26625			
115 ->122	-0.15934			
119 ->124	0.36842			
119 ->130	-0.17466			
Excited State 25:	Singlet	4.7649 eV	260.20 nm	f=0.0147
109 ->121	0.16220			
114 ->122	0.16451			
116 ->124	0.28489			
116 ->130	-0.18533			
117 ->124	0.13708			
117 ->130	-0.10022			
118 ->123	-0.11171			
118 ->124	0.35069			
118 ->130	-0.17161			
120 ->126	0.10659			
Excited State 26:	Singlet	4.8755 eV	254.30 nm	f=0.0057
109 ->122	-0.11401			
111 ->122	-0.21166			
112 ->122	0.37460			
113 ->122	0.28320			
114 ->122	-0.11173			
119 ->123	0.32123			
120 ->125	0.14255			
120 ->127	-0.13085			

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Excited State 27: Singlet 4.9168 eV 252.17 nm f=0.0046
112 ->122 -0.11160
119 ->123 -0.10865
120 ->125 0.66914

Excited State 28: Singlet 4.9369 eV 251.14 nm f=0.0090
111 ->122 -0.19332
113 ->122 -0.33977
115 ->122 -0.13559
119 ->123 0.39110
119 ->124 0.17543
120 ->127 0.19025

Excited State 29: Singlet 4.9698 eV 249.47 nm f=0.1480
120 ->126 0.64289
120 ->127 -0.10468

Excited State 30: Singlet 5.0285 eV 246.56 nm f=0.2704
111 ->122 -0.17633
113 ->122 0.21065
115 ->122 0.16546
120 ->124 0.12457
120 ->126 0.15608
120 ->127 0.48076
120 ->130 0.13208

Excited State 31: Singlet 5.0439 eV 245.81 nm f=0.0080
111 ->122 -0.17502
112 ->122 0.42213
113 ->122 -0.26066
114 ->122 0.11675
115 ->122 -0.20715
119 ->123 -0.32355
119 ->124 -0.11750
120 ->127 0.10303

Excited State 32: Singlet 5.1079 eV 242.73 nm f=0.0499
111 ->122 0.46905
112 ->122 0.23147
114 ->122 0.17906
115 ->122 -0.10832
119 ->123 0.18067
120 ->127 0.13663
120 ->128 -0.15040

Excited State 33: Singlet 5.1799 eV 239.35 nm f=0.0680
113 ->124 -0.12221
115 ->124 0.11983
117 ->124 0.12898
120 ->124 -0.11718
120 ->127 0.19555
120 ->128 0.34815
120 ->129 0.29165
120 ->130 -0.20326

Excited State 34: Singlet 5.2241 eV 237.33 nm f=0.0057
109 ->122 0.14332
110 ->122 0.24783
111 ->124 -0.10659
113 ->122 0.12667
113 ->124 0.12654

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115 ->124	-0.10376
117 ->124	-0.20414
119 ->126	-0.13685
120 ->127	0.12619
120 ->128	0.26417
120 ->129	0.17788

Excited State 35: Singlet 5.2432 eV 236.47 nm f=0.0167

109 ->122	-0.17120
110 ->122	-0.29203
113 ->124	0.15556
117 ->124	-0.16007
117 ->130	0.10507
119 ->126	0.18977
120 ->128	-0.12366
120 ->129	0.30695

Excited State 36: Singlet 5.2617 eV 235.63 nm f=0.0167

109 ->122	-0.18056
110 ->122	-0.28403
118 ->123	-0.16202
119 ->126	-0.13229
120 ->128	0.35398
120 ->129	-0.26293
120 ->130	0.14063

Excited State 37: Singlet 5.3151 eV 233.27 nm f=0.0428

118 ->125	-0.12133
119 ->125	0.56950
119 ->126	0.18210
119 ->127	0.10405
120 ->130	-0.11321

Excited State 38: Singlet 5.3442 eV 232.00 nm f=0.0246

109 ->122	-0.11202
110 ->122	-0.15652
111 ->122	0.15020
116 ->123	0.15224
117 ->123	0.17297
118 ->123	0.50507
118 ->124	0.11109
119 ->125	0.10763
119 ->126	-0.15639

Excited State 39: Singlet 5.3468 eV 231.88 nm f=0.0976

118 ->123	0.11333
119 ->125	-0.21187
119 ->126	0.35479
119 ->127	0.20074
119 ->128	-0.11711
120 ->128	0.15939
120 ->129	-0.31211
120 ->130	-0.10752

Excited State 40: Singlet 5.3726 eV 230.77 nm f=0.0047

117 ->124	0.14650
118 ->123	0.14052
119 ->126	0.20382
120 ->124	0.13986
120 ->127	-0.16660
120 ->128	0.16502
120 ->129	0.24950

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120 ->130 0.41673
120 ->132 0.10413

Excited State 41: Singlet 5.4397 eV 227.93 nm f=0.0146
107 ->122 -0.13085
119 ->124 0.19395
119 ->126 -0.29293
119 ->127 0.45557
119 ->130 0.15283

PYPdON: D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 3.0974 eV 400.28 nm f=0.0612
112 ->114 0.12185
113 ->114 0.66011

Excited State 2: Singlet 3.2759 eV 378.47 nm f=0.1114
112 ->115 0.10047
113 ->114 -0.10679
113 ->115 0.63570
113 ->117 0.10403

Excited State 3: Singlet 3.5319 eV 351.04 nm f=0.0044
110 ->114 0.16357
111 ->114 0.63081
112 ->114 0.13142
113 ->117 0.13690

Excited State 4: Singlet 3.5911 eV 345.25 nm f=0.0041
110 ->117 -0.11467
111 ->117 -0.19549
112 ->114 0.45006
112 ->115 -0.11744
112 ->117 -0.14690
113 ->115 0.12771
113 ->117 -0.31505

Excited State 5: Singlet 3.6165 eV 342.82 nm f=0.0359
103 ->117 0.11822
111 ->114 -0.18620
111 ->117 -0.16753
112 ->114 0.30265
112 ->117 0.11239
113 ->114 -0.11022
113 ->117 0.45021
113 ->120 -0.11337

Excited State 6: Singlet 3.7517 eV 330.48 nm f=0.0148
113 ->116 0.67813

Excited State 7: Singlet 3.7686 eV 328.99 nm f=0.0450
110 ->115 0.17116
111 ->115 0.51393
111 ->117 0.20445
112 ->114 0.24903
112 ->115 0.20526

Excited State 8: Singlet 3.8704 eV 320.34 nm f=0.0203
110 ->117 0.12496

111 ->114 -0.13095
111 ->115 -0.38335
111 ->117 0.38758
111 ->120 -0.11317
112 ->114 0.20096
112 ->117 0.12569

Excited State 9: Singlet 4.0260 eV 307.96 nm f=0.1479
106 ->117 -0.12738
109 ->114 -0.10536
110 ->114 -0.16942
111 ->115 -0.13997
111 ->117 -0.21233
112 ->115 0.50386
112 ->117 0.16162

Excited State 10: Singlet 4.1110 eV 301.59 nm f=0.0628
106 ->117 -0.25882
108 ->117 -0.13216
110 ->114 0.12599
112 ->115 -0.24029
112 ->117 0.42942
112 ->120 -0.10733
113 ->117 -0.13745

Excited State 11: Singlet 4.1261 eV 300.49 nm f=0.0370
110 ->114 0.57822
110 ->115 0.13804
111 ->114 -0.14418
112 ->115 0.19922
112 ->116 0.13233

Excited State 12: Singlet 4.2243 eV 293.50 nm f=0.0210
106 ->114 -0.11699
109 ->114 0.46066
110 ->115 0.22452
111 ->116 0.11099
112 ->116 -0.36645

Excited State 13: Singlet 4.2894 eV 289.05 nm f=0.0020
110 ->116 0.16168
111 ->116 0.62528
112 ->116 0.20354

Excited State 14: Singlet 4.3269 eV 286.54 nm f=0.0583
107 ->115 0.11617
109 ->114 -0.22672
109 ->115 0.18897
110 ->114 -0.12143
110 ->115 0.51844
111 ->115 -0.11306
112 ->115 -0.13008
113 ->122 0.10380

Excited State 15: Singlet 4.3772 eV 283.25 nm f=0.0132
107 ->114 0.38909
107 ->115 0.12441
108 ->114 0.30168
108 ->115 0.11940
109 ->114 0.20501
110 ->114 -0.13683
112 ->116 0.31104

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Excited State 16: Singlet 4.4405 eV 279.21 nm f=0.0462
104 ->117 0.44379
104 ->120 -0.15683
105 ->117 0.12562
106 ->114 -0.13627
107 ->115 0.10090
107 ->117 0.23962
109 ->114 -0.11981
109 ->117 0.13319
112 ->116 -0.13500

Excited State 17: Singlet 4.4633 eV 277.79 nm f=0.0318
104 ->117 0.20552
106 ->114 0.31750
107 ->114 -0.19589
107 ->115 -0.12653
107 ->117 0.13935
109 ->114 0.23426
111 ->116 -0.12608
112 ->116 0.20828
113 ->118 -0.25687

Excited State 18: Singlet 4.4935 eV 275.92 nm f=0.0072
106 ->114 0.16562
112 ->116 0.10644
113 ->118 0.62759

Excited State 19: Singlet 4.5522 eV 272.36 nm f=0.1321
104 ->114 -0.12355
106 ->114 0.28305
108 ->114 0.45295
108 ->115 0.21384
109 ->114 -0.13774
111 ->116 0.11703
112 ->116 -0.20531

Excited State 20: Singlet 4.5871 eV 270.29 nm f=0.0376
106 ->115 -0.16959
107 ->114 -0.24826
107 ->115 0.35341
108 ->114 -0.11204
108 ->115 0.29389
109 ->115 0.32198
110 ->115 -0.14960

Excited State 21: Singlet 4.6486 eV 266.71 nm f=0.0471
106 ->115 0.26404
107 ->115 -0.25210
109 ->115 0.52720
110 ->115 -0.10976
Excited State 21: Singlet 4.6486 eV 266.71 nm f=0.0471
106 ->115 0.26404
107 ->115 -0.25210
109 ->115 0.52720
110 ->115 -0.10976

Excited State 22: Singlet 4.7154 eV 262.93 nm f=0.0818
104 ->114 0.14056
106 ->114 0.32565
106 ->115 -0.13158
107 ->114 0.17648

107 ->115 0.12523
108 ->115 -0.26716
109 ->115 0.12656
109 ->116 -0.15538
112 ->116 -0.16082
113 ->117 0.14848
113 ->120 0.18533

Excited State 23: Singlet 4.7373 eV 261.72 nm f=0.0330
104 ->114 0.32493
106 ->114 0.19895
106 ->115 0.16451
106 ->117 0.10308
107 ->114 0.22164
108 ->114 -0.27100
108 ->115 0.32248
113 ->117 -0.10531

Excited State 24: Singlet 4.7851 eV 259.10 nm f=0.0083
109 ->116 0.20746
110 ->116 0.59627
111 ->116 -0.14160

Excited State 25: Singlet 4.8215 eV 257.15 nm f=0.0150
106 ->115 -0.25402
106 ->117 0.17190
108 ->115 -0.22888
108 ->117 0.11789
109 ->117 0.13143
110 ->116 0.19322
110 ->117 0.25831
111 ->117 -0.15091
112 ->117 0.13486
113 ->117 -0.22988
113 ->120 -0.13107

Excited State 26: Singlet 4.8798 eV 254.08 nm f=0.0152
104 ->114 -0.14795
104 ->115 0.14964
106 ->115 0.27256
107 ->115 0.26705
108 ->115 -0.14204
109 ->116 0.23665
110 ->116 -0.12990
110 ->117 0.13012
112 ->117 0.12039
113 ->119 -0.20543
113 ->120 0.24795

Excited State 27: Singlet 4.9414 eV 250.91 nm f=0.0078
104 ->114 0.38011
105 ->114 0.27984
105 ->115 0.22517
107 ->114 -0.23409
108 ->114 0.20059
108 ->115 -0.10974
112 ->118 0.16645

Excited State 28: Singlet 4.9628 eV 249.83 nm f=0.0685
104 ->114 0.14089
106 ->114 0.11347
106 ->115 -0.24602

107 ->115 -0.10777
109 ->116 0.48529
110 ->116 -0.10189
113 ->119 -0.19256
113 ->120 -0.14307

Excited State 29: Singlet 4.9947 eV 248.23 nm f=0.0035
103 ->114 0.11681
104 ->114 0.31836
104 ->115 0.10265
105 ->114 -0.23025
105 ->115 -0.25649
106 ->114 -0.12152
107 ->114 -0.10825
107 ->115 0.15443
108 ->114 0.15024
108 ->115 -0.10622
108 ->118 -0.11175
109 ->116 -0.15502
111 ->118 -0.13887
112 ->118 -0.28360

Excited State 30: Singlet 5.0201 eV 246.97 nm f=0.0131
104 ->115 -0.24270
106 ->115 -0.17117
107 ->115 -0.12150
110 ->117 0.19104
113 ->120 0.48258
113 ->122 0.17191

Excited State 31: Singlet 5.0339 eV 246.29 nm f=0.2724
109 ->116 0.21035
113 ->119 0.57143

Excited State 32: Singlet 5.1085 eV 242.70 nm f=0.0137
103 ->114 -0.25973
105 ->114 0.43595
105 ->115 -0.13236
111 ->118 -0.16077
112 ->118 -0.29738
113 ->121 -0.14728

Excited State 33: Singlet 5.1138 eV 242.45 nm f=0.0261
104 ->115 0.10728
105 ->114 0.11988
112 ->118 -0.14614
113 ->121 0.61850

Excited State 34: Singlet 5.1721 eV 239.71 nm f=0.0309
104 ->115 -0.26499
105 ->115 -0.12910
106 ->116 -0.15897
107 ->115 0.11379
107 ->116 0.28064
108 ->116 0.14889
109 ->117 0.11468
110 ->117 -0.21789
112 ->118 0.22151
113 ->122 -0.27889

Excited State 35: Singlet 5.1851 eV 239.11 nm f=0.0131
104 ->115 0.22737

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106 ->116 -0.12677
107 ->116 0.42563
108 ->116 0.33399
109 ->117 -0.14633
110 ->117 0.16389
113 ->122 0.12782

PYPtON: D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 2.9174 eV 424.98 nm f=0.0455
112 ->114 -0.13519
113 ->114 0.66500

Excited State 2: Singlet 3.1315 eV 395.92 nm f=0.0809
112 ->114 0.17774
112 ->115 -0.12143
113 ->115 0.64006

Excited State 3: Singlet 3.4653 eV 357.78 nm f=0.1216
111 ->114 0.21776
112 ->114 0.58128
112 ->115 -0.10995
113 ->114 0.12938
113 ->115 -0.19208
113 ->116 0.11781

Excited State 4: Singlet 3.4880 eV 355.45 nm f=0.0196
110 ->114 0.13310
111 ->114 0.64542
112 ->114 -0.20088

Excited State 5: Singlet 3.6360 eV 340.99 nm f=0.0260
113 ->116 0.67816

Excited State 6: Singlet 3.7337 eV 332.06 nm f=0.0025
110 ->115 0.14958
111 ->115 0.67407

Excited State 7: Singlet 3.8321 eV 323.54 nm f=0.2055
112 ->114 0.12831
112 ->115 0.63819

Excited State 8: Singlet 4.0515 eV 306.02 nm f=0.0398
110 ->114 0.60207
111 ->114 -0.11558
112 ->116 -0.24497

Excited State 9: Singlet 4.1112 eV 301.57 nm f=0.0150
106 ->114 0.11443
109 ->114 0.46144
110 ->115 0.20544
112 ->116 0.39783

Excited State 10: Singlet 4.2193 eV 293.85 nm f=0.0052
113 ->118 0.55630
113 ->122 -0.28583

Excited State 11: Singlet 4.2681 eV 290.49 nm f=0.0307
105 ->114 0.12563
106 ->114 0.25644

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107 ->114	0.29356			
109 ->114	0.31566			
110 ->114	-0.15669			
110 ->115	-0.22524			
112 ->116	-0.30043			
113 ->118	0.10150			
113 ->121	-0.10822			
Excited State 12:	Singlet	4.3097 eV	287.68 nm	f=0.0022
106 ->114	-0.16673			
107 ->114	-0.13895			
109 ->115	-0.13365			
110 ->115	-0.21267			
110 ->116	0.10678			
111 ->115	0.10594			
111 ->116	0.56891			
Excited State 13:	Singlet	4.3173 eV	287.18 nm	f=0.0111
106 ->114	0.20470			
107 ->114	0.18077			
108 ->114	-0.12903			
109 ->114	-0.14658			
109 ->115	0.19289			
110 ->115	0.38153			
111 ->116	0.36279			
Excited State 14:	Singlet	4.3475 eV	285.19 nm	f=0.0104
106 ->114	-0.17651			
107 ->114	-0.15185			
108 ->114	0.39344			
109 ->114	0.24808			
109 ->115	0.12399			
110 ->114	-0.14408			
110 ->115	0.20645			
112 ->116	-0.24017			
113 ->117	-0.20803			
Excited State 15:	Singlet	4.3769 eV	283.27 nm	f=0.0027
108 ->114	0.16238			
113 ->117	0.65263			
Excited State 16:	Singlet	4.4705 eV	277.34 nm	f=0.1451
106 ->114	0.26536			
107 ->114	0.15455			
108 ->114	0.46055			
108 ->115	0.17984			
109 ->114	-0.16814			
109 ->115	-0.16861			
112 ->116	0.19594			
Excited State 17:	Singlet	4.5300 eV	273.69 nm	f=0.1211
105 ->115	0.12622			
106 ->115	0.28696			
107 ->115	0.26879			
109 ->115	0.38747			
110 ->115	-0.25387			
113 ->118	-0.10400			
113 ->119	-0.12068			
Excited State 18:	Singlet	4.5992 eV	269.58 nm	f=0.0690
104 ->114	0.10785			
106 ->115	-0.24521			

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107 ->115 -0.27877
108 ->115 0.32405
109 ->115 0.36524
111 ->118 0.10771

Excited State 19: Singlet 4.6305 eV 267.75 nm f=0.0829
104 ->114 0.23425
105 ->114 0.14851
106 ->114 -0.29902
106 ->115 -0.14498
107 ->114 0.32792
108 ->115 -0.15325
109 ->115 0.13177
109 ->116 -0.11791
111 ->118 -0.14269
111 ->122 0.11974
112 ->116 0.13002
113 ->119 -0.10877

Excited State 20: Singlet 4.6739 eV 265.27 nm f=0.0107
104 ->114 0.15977
106 ->114 -0.18049
107 ->114 0.12478
107 ->115 0.13722
108 ->115 0.10328
109 ->115 -0.15492
111 ->118 0.39112
111 ->122 -0.31933

Excited State 21: Singlet 4.7362 eV 261.78 nm f=0.0044
104 ->114 0.20696
105 ->114 0.11473
106 ->114 -0.14676
106 ->115 0.26716
107 ->115 0.17170
108 ->115 0.29004
111 ->118 -0.12234
112 ->118 0.32430
112 ->122 -0.17729

Excited State 22: Singlet 4.7621 eV 260.35 nm f=0.0107
107 ->115 0.13629
108 ->114 -0.10068
108 ->115 0.34337
109 ->116 0.24702
110 ->116 0.17076
111 ->118 -0.13370
112 ->118 -0.25983
112 ->122 0.16727
113 ->119 -0.15748

Excited State 23: Singlet 4.8059 eV 257.98 nm f=0.0112
108 ->115 -0.15668
109 ->116 0.11521
110 ->116 0.57232
111 ->116 -0.10005
111 ->118 0.11502
112 ->118 0.13979
113 ->121 -0.10575

Excited State 24: Singlet 4.8625 eV 254.98 nm f=0.0201
105 ->114 -0.33876

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105 ->115 -0.21903
106 ->115 0.11285
107 ->114 0.19395
112 ->117 0.42009
112 ->118 0.11108
113 ->119 -0.14870

Excited State 25: Singlet 4.8704 eV 254.57 nm f=0.1185
104 ->115 -0.13721
106 ->115 0.24165
107 ->115 -0.14832
109 ->116 -0.24886
110 ->116 0.27766
112 ->118 -0.19564
113 ->119 0.28438
113 ->120 -0.14000

Excited State 26: Singlet 4.9114 eV 252.44 nm f=0.0249
104 ->114 -0.22048
105 ->114 -0.21413
107 ->114 0.11266
108 ->115 0.16039
109 ->116 -0.23218
112 ->117 -0.15207
112 ->118 0.10670
113 ->118 -0.16728
113 ->119 0.22099
113 ->120 0.28275
113 ->121 -0.15837
113 ->122 -0.21018

Excited State 27: Singlet 4.9246 eV 251.76 nm f=0.0323
104 ->114 0.28665
104 ->115 0.16724
106 ->114 0.17838
106 ->115 -0.10072
107 ->114 -0.19231
107 ->115 0.11100
112 ->117 0.34605
113 ->119 0.30203
113 ->120 0.14751

Excited State 28: Singlet 4.9522 eV 250.36 nm f=0.0411
104 ->115 -0.19414
105 ->114 0.11850
106 ->115 0.18019
107 ->115 -0.20882
109 ->116 0.36857
113 ->119 0.16404
113 ->120 0.31379
113 ->121 0.13940
113 ->122 -0.10442

Excited State 29: Singlet 4.9852 eV 248.70 nm f=0.3972
104 ->114 -0.10631
104 ->115 0.19270
105 ->114 -0.14943
106 ->115 -0.12188
107 ->114 0.19822
107 ->115 0.11180
109 ->116 0.26545
113 ->118 0.14385

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113 ->119 0.33955
113 ->120 -0.13231
113 ->122 0.18565

Excited State 30: Singlet 5.0162 eV 247.17 nm f=0.0046
103 ->114 0.13791
104 ->114 0.36426
105 ->114 -0.34238
105 ->115 -0.14298
106 ->114 0.11886
106 ->115 0.10755
112 ->117 -0.35073

Excited State 31: Singlet 5.0446 eV 245.77 nm f=0.1339
109 ->116 -0.13165
113 ->118 0.16667
113 ->120 0.41652
113 ->121 0.32637
113 ->122 0.28668

Excited State 32: Singlet 5.1256 eV 241.89 nm f=0.0259
103 ->114 0.15036
104 ->115 0.22137
105 ->115 0.30440
106 ->116 -0.10981
107 ->115 -0.21055
111 ->117 0.28526
113 ->120 -0.11186
113 ->121 0.19838
113 ->122 -0.19091

Excited State 33: Singlet 5.1403 eV 241.20 nm f=0.0025
103 ->114 0.17163
104 ->115 -0.24600
105 ->114 -0.10156
111 ->117 0.50670
113 ->121 -0.21120
113 ->122 0.13782

Excited State 34: Singlet 5.1778 eV 239.45 nm f=0.0070
103 ->114 -0.16960
103 ->115 0.10675
105 ->115 -0.13816
105 ->116 0.12780
106 ->116 0.31448
107 ->115 0.11121
107 ->116 0.28015
108 ->116 -0.25279
111 ->117 0.20774
113 ->121 0.20778
113 ->122 -0.13434

Excited State 35: Singlet 5.1862 eV 239.06 nm f=0.0368
103 ->114 -0.17077
104 ->115 0.25414
105 ->115 0.19157
106 ->115 0.16673
106 ->116 0.17000
107 ->115 -0.25368
107 ->116 0.18775
113 ->120 0.11037
113 ->121 -0.28824

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113 ->122 0.14960

BEPdON: D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 2.9680 eV 417.73 nm f=0.0312
119 ->120 0.67436

Excited State 2: Singlet 3.2738 eV 378.72 nm f=0.1042
119 ->121 0.63010
119 ->123 0.13810

Excited State 3: Singlet 3.4570 eV 358.65 nm f=0.0073
116 ->120 0.29789
117 ->120 0.44835
117 ->123 -0.12133
118 ->120 0.36139
119 ->122 0.11078

Excited State 4: Singlet 3.4779 eV 356.49 nm f=0.0109
115 ->120 0.10060
116 ->120 -0.20588
117 ->120 -0.35991
118 ->120 0.48568
119 ->120 0.10649
119 ->122 0.16018

Excited State 5: Singlet 3.5509 eV 349.16 nm f=0.0117
110 ->123 -0.10169
111 ->123 -0.14469
118 ->123 -0.13428
119 ->121 -0.14717
119 ->122 0.15446
119 ->123 0.54779
119 ->126 -0.14061

Excited State 6: Singlet 3.6895 eV 336.05 nm f=0.1018
115 ->120 0.10503
118 ->120 -0.23660
119 ->122 0.59501
119 ->123 -0.10427

Excited State 7: Singlet 3.7236 eV 332.97 nm f=0.0049
116 ->121 0.18392
116 ->123 0.28156
117 ->121 0.29683
117 ->123 0.35184
117 ->126 -0.10144
118 ->120 0.13070
118 ->121 -0.11157
119 ->122 0.16338

Excited State 8: Singlet 3.8425 eV 322.66 nm f=0.0332
116 ->120 0.25460
116 ->121 0.30195
116 ->123 -0.14745
117 ->120 -0.18902
117 ->121 0.43054
117 ->123 -0.16669

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Excited State	9:	Singlet	3.8623 eV	321.01 nm f=0.0936
116 ->120	0.46096			
116 ->121	-0.19289			
117 ->120	-0.24827			
117 ->121	-0.21218			
117 ->123	0.16472			
118 ->121	-0.18161			
Excited State	10:	Singlet	4.0206 eV	308.37 nm f=0.0461
112 ->123	-0.21875			
116 ->120	0.14852			
116 ->123	0.21556			
118 ->121	0.40207			
118 ->123	0.30192			
Excited State	11:	Singlet	4.0684 eV	304.75 nm f=0.0775
112 ->123	0.20478			
116 ->123	-0.11171			
117 ->123	0.14211			
118 ->121	0.47191			
118 ->123	-0.28067			
118 ->123	0.30192			
Excited State	12:	Singlet	4.1190 eV	301.00 nm f=0.0020
112 ->120	0.10132			
115 ->120	0.53259			
116 ->120	-0.11338			
116 ->121	0.11997			
117 ->122	-0.13299			
118 ->122	-0.28837			
119 ->122	-0.12799			
Excited State	13:	Singlet	4.1956 eV	295.51 nm f=0.0143
116 ->122	0.31236			
117 ->122	0.57342			
118 ->122	-0.17215			
Excited State	14:	Singlet	4.2303 eV	293.08 nm f=0.1944
113 ->120	0.18029			
115 ->120	-0.21721			
115 ->122	-0.11325			
116 ->121	0.41640			
116 ->122	-0.21076			
117 ->121	-0.29628			
118 ->122	-0.14602			
Excited State	15:	Singlet	4.2989 eV	288.41 nm f=0.0159
113 ->120	0.52713			
113 ->121	-0.12723			
114 ->120	0.15460			
115 ->120	0.14609			
118 ->122	0.31746			
Excited State	16:	Singlet	4.3378 eV	285.82 nm f=0.0353
112 ->120	0.15186			
113 ->120	-0.27263			
116 ->120	0.10914			
116 ->121	0.27066			
116 ->122	0.21130			
117 ->121	-0.19225			
118 ->122	0.37873			

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Excited State 17:	Singlet	4.3806 eV	283.03 nm	f=0.0163
109 ->123	0.47120			
109 ->126	-0.17599			
110 ->123	0.12835			
113 ->123	-0.26056			
114 ->120	-0.12023			
116 ->123	0.12025			
Excited State 18:	Singlet	4.4197 eV	280.52 nm	f=0.0189
111 ->120	-0.10063			
112 ->120	0.28513			
114 ->120	0.29141			
114 ->121	-0.12410			
115 ->120	-0.21620			
115 ->122	0.22089			
116 ->122	0.25549			
117 ->122	-0.13412			
118 ->122	-0.19220			
118 ->125	0.10416			
119 ->125	-0.11001			
Excited State 19:	Singlet	4.4574 eV	278.15 nm	f=0.0024
113 ->121	0.10203			
114 ->120	0.13045			
119 ->124	0.65053			
Excited State 20:	Singlet	4.5081 eV	275.02 nm	f=0.0215
110 ->120	0.17918			
111 ->120	0.26529			
112 ->120	0.16421			
113 ->121	0.22057			
114 ->120	0.34353			
115 ->121	0.10189			
115 ->122	-0.10736			
116 ->122	-0.15636			
117 ->122	0.10467			
119 ->124	-0.21358			
119 ->125	0.16618			
Excited State 21:	Singlet	4.5516 eV	272.40 nm	f=0.0048
109 ->120	-0.13162			
113 ->120	0.22129			
113 ->121	0.49816			
114 ->120	-0.17431			
114 ->121	0.20262			
115 ->121	0.16062			
Excited State 22:	Singlet	4.6378 eV	267.33 nm	f=0.0432
109 ->120	-0.20078			
111 ->120	0.13233			
112 ->120	0.25437			
113 ->121	-0.16897			
114 ->120	-0.29276			
114 ->121	-0.11693			
115 ->121	0.20443			
119 ->125	0.33663			
119 ->126	0.11337			
Excited State 23:	Singlet	4.6639 eV	265.83 nm	f=0.0610
114 ->120	-0.10048			
114 ->121	-0.21867			
115 ->121	0.37353			

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115 ->122 0.11790
116 ->122 -0.19667
117 ->122 0.14041
119 ->123 -0.12449
119 ->125 -0.33276

Excited State 24: Singlet 4.6693 eV 265.53 nm f=0.0012
109 ->120 -0.10983
111 ->120 0.21992
112 ->120 0.36711
114 ->120 -0.13519
114 ->121 0.14137
115 ->121 -0.30871
115 ->122 0.14146
116 ->122 -0.18643
117 ->122 0.12618
119 ->125 -0.20436

Excited State 25: Singlet 4.6928 eV 264.20 nm f=0.0244
111 ->123 0.11062
112 ->123 0.14114
114 ->121 0.19537
115 ->121 0.27106
116 ->122 -0.15325
116 ->123 -0.20655
117 ->123 0.17655
118 ->123 0.28198
119 ->123 0.19022
119 ->126 0.14556

Excited State 26: Singlet 4.7587 eV 260.54 nm f=0.0072
110 ->120 0.22936
111 ->120 0.36712
112 ->120 -0.18238
115 ->122 -0.14019
116 ->122 0.24073
117 ->122 -0.17191
118 ->123 0.15787
119 ->125 -0.24415

Excited State 27: Singlet 4.7780 eV 259.49 nm f=0.0040
109 ->120 0.16945
110 ->121 0.11094
111 ->121 0.10828
113 ->121 -0.17450
114 ->121 0.42768
115 ->121 0.13801
116 ->123 0.14342
117 ->123 -0.17069
118 ->123 -0.21756
119 ->126 0.16200

Excited State 28: Singlet 4.8882 eV 253.64 nm f=0.0043
109 ->120 0.55451
110 ->120 0.17101
112 ->120 0.12251
113 ->120 0.13213
114 ->120 -0.24963
114 ->121 -0.11209

Excited State 29: Singlet 4.9032 eV 252.86 nm f=0.1190
110 ->120 0.16031
111 ->120 0.12208

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111 ->121 -0.10204
112 ->120 -0.19384
115 ->122 0.37825
118 ->124 0.11886
118 ->125 0.26839
119 ->125 0.25360

Excited State 30: Singlet 4.9165 eV 252.18 nm f=0.0040
112 ->121 -0.22425
114 ->121 -0.12556
115 ->121 -0.14170
118 ->123 -0.10523
119 ->123 0.16923
119 ->125 -0.13471
119 ->126 0.51268
119 ->128 -0.11024

Excited State 31: Singlet 4.9787 eV 249.03 nm f=0.0001
109 ->120 -0.15362
110 ->120 0.31686
110 ->121 -0.26350
111 ->120 -0.20553
111 ->121 0.13668
112 ->121 -0.12875
114 ->124 -0.12928
117 ->124 0.23710
118 ->124 -0.30687

Excited State 32: Singlet 5.0148 eV 247.23 nm f=0.0037
109 ->121 -0.20451
111 ->121 0.25744
112 ->121 0.40058
113 ->121 0.13060
113 ->122 0.17480
114 ->121 -0.14334
117 ->123 -0.11404
118 ->124 -0.13794
119 ->127 0.11786

Excited State 33: Singlet 5.0549 eV 245.28 nm f=0.0359
112 ->121 -0.19079
113 ->122 0.50280
114 ->122 0.22952
118 ->124 0.10686
119 ->126 -0.10960
119 ->127 -0.21478

Excited State 34: Singlet 5.0645 eV 244.81 nm f=0.0190
110 ->120 0.34142
110 ->121 0.17774
111 ->120 -0.20934
111 ->121 0.20935
113 ->122 -0.21958
118 ->124 0.33725
119 ->127 -0.16661

Excited State 35: Singlet 5.0768 eV 244.22 nm f=0.0300
110 ->120 -0.25376
110 ->121 0.11864
111 ->120 0.17214
111 ->121 0.30035
112 ->121 -0.13562

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113 ->122 -0.18511
117 ->124 0.18390
118 ->124 -0.13506
118 ->125 0.16086
119 ->127 -0.21371

Excited State 36: Singlet 5.1070 eV 242.77 nm f=0.0053
111 ->121 -0.13954
112 ->121 0.10664
112 ->122 -0.10558
114 ->122 -0.10701
119 ->127 -0.50947
119 ->128 -0.30224
Excited State 37: Singlet 5.1178 eV 242.26 nm f=0.0581
110 ->121 -0.21666
112 ->122 0.26535
114 ->122 0.25863
115 ->122 -0.17936
117 ->124 0.28574
118 ->124 0.28299
119 ->128 -0.10236

Excited State 38: Singlet 5.1407 eV 241.18 nm f=0.0401
109 ->121 -0.24735
112 ->122 -0.20726
113 ->122 0.21345
113 ->123 -0.10070
114 ->122 -0.18359
116 ->123 -0.10660
116 ->124 0.12208
116 ->125 0.11881
117 ->123 0.13374
117 ->124 0.18988
117 ->125 0.13697
118 ->124 0.14953
118 ->125 -0.17836
119 ->126 0.17038

Excited State 39: Singlet 5.1548 eV 240.52 nm f=0.0226
109 ->121 -0.25022
110 ->123 -0.11034
111 ->123 -0.13035
112 ->122 0.17667
112 ->123 -0.10701
114 ->122 0.19075
116 ->124 -0.15324
117 ->123 0.10938
117 ->124 -0.30181
118 ->124 -0.21242
118 ->125 0.11812
119 ->126 0.16201
119 ->128 0.10423

Excited State 40: Singlet 5.2030 eV 238.29 nm f=0.0072
109 ->121 0.10992
110 ->121 0.26610
111 ->121 -0.16305
112 ->122 0.13433
114 ->124 0.12157
116 ->124 0.11420
116 ->125 0.20795
117 ->125 0.42115

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118 ->124 -0.19302
119 ->128 -0.13703

BEPtON: D95V/SDD/mPW1PW91 level of theory

Excited State 1: Singlet 2.7951 eV 443.58 nm f=0.0285
118 ->120 -0.11940
119 ->120 0.67000

Excited State 2: Singlet 3.1228 eV 397.02 nm f=0.0754
118 ->120 -0.18097
119 ->121 0.63690

Excited State 3: Singlet 3.3332 eV 371.97 nm f=0.0476
118 ->120 0.59743
119 ->120 0.12928
119 ->121 0.21088
119 ->122 0.21626

Excited State 4: Singlet 3.4073 eV 363.87 nm f=0.0037
116 ->120 0.36634
117 ->120 0.58516

Excited State 5: Singlet 3.5780 eV 346.52 nm f=0.1782
118 ->120 -0.23280
119 ->122 0.62574

Excited State 6: Singlet 3.7353 eV 331.92 nm f=0.0051
116 ->120 -0.13949
116 ->121 0.38507
117 ->121 0.54335

Excited State 7: Singlet 3.7655 eV 329.26 nm f=0.1270
115 ->122 -0.11430
116 ->120 0.48942
116 ->121 0.12182
117 ->120 -0.29337
117 ->121 0.15497
118 ->121 0.26045
118 ->122 0.10751

Excited State 8: Singlet 3.8961 eV 318.22 nm f=0.1769
116 ->120 -0.18514
117 ->120 0.13139
118 ->121 0.58960
118 ->122 -0.15606

Excited State 9: Singlet 4.0725 eV 304.44 nm f=0.0393
112 ->120 -0.11544
113 ->120 0.12965
115 ->120 0.10876
116 ->120 -0.13161
116 ->121 0.31797
117 ->121 -0.20384
118 ->122 0.46798

Excited State 10: Singlet 4.1093 eV 301.71 nm f=0.0209
112 ->120 0.12277
114 ->120 0.11589

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115 ->120 0.56958
116 ->122 0.14781
117 ->122 -0.20721
119 ->124 0.14861

Excited State 11: Singlet 4.1714 eV 297.22 nm f=0.0070
113 ->120 -0.19070
114 ->120 0.11826
115 ->120 -0.16667
116 ->122 -0.11957
117 ->122 -0.10520
119 ->124 0.44896
119 ->125 -0.21231
119 ->128 0.20495
119 ->129 -0.15347

Excited State 12: Singlet 4.2104 eV 294.47 nm f=0.0208
111 ->120 0.17455
113 ->120 -0.30170
114 ->120 0.19305
116 ->121 -0.23407
116 ->122 0.12914
117 ->121 0.18641
117 ->122 0.20851
118 ->122 0.32556

Excited State 13: Singlet 4.2284 eV 293.22 nm f=0.0153
111 ->120 0.15068
114 ->120 0.26007
116 ->121 0.30391
116 ->122 0.25978
117 ->121 -0.19671
117 ->122 0.32807
118 ->122 -0.18964

Excited State 14: Singlet 4.2337 eV 292.85 nm f=0.0056
111 ->120 -0.19217
113 ->120 0.15843
114 ->120 -0.27028
116 ->121 -0.10608
116 ->122 0.25279
117 ->121 0.12983
117 ->122 0.38589
119 ->124 0.23396

Excited State 15: Singlet 4.3329 eV 286.14 nm f=0.0011
119 ->123 0.68012

Excited State 16: Singlet 4.3805 eV 283.03 nm f=0.0623
113 ->120 0.46367
114 ->120 0.38237
114 ->121 -0.15665
115 ->120 -0.14666
115 ->121 0.10098
116 ->121 -0.10060
118 ->122 0.10047

Excited State 17: Singlet 4.4059 eV 281.40 nm f=0.0090
111 ->120 -0.21659
112 ->120 0.25713
115 ->120 -0.19009

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115 ->122 0.18641
116 ->121 0.11111
116 ->122 0.30004
117 ->122 -0.17973
118 ->122 0.16748
119 ->125 0.24288

Excited State 18: Singlet 4.5307 eV 273.65 nm f=0.0100
109 ->120 -0.16413
111 ->120 0.10661
111 ->121 -0.30391
112 ->121 -0.17082
113 ->121 0.39487
114 ->120 -0.11402
114 ->121 -0.31441
119 ->124 0.10907

Excited State 19: Singlet 4.5687 eV 271.37 nm f=0.0338
109 ->120 0.12700
112 ->120 -0.27336
115 ->121 -0.28446
118 ->125 -0.10245
119 ->124 0.27896
119 ->125 0.32665
119 ->127 0.14005

Excited State 20: Singlet 4.5911 eV 270.05 nm f=0.0101
111 ->120 0.29997
112 ->120 0.13579
113 ->120 0.14572
114 ->121 0.36510
116 ->124 0.14585
116 ->128 0.12533
117 ->124 0.16431
117 ->125 -0.11201
117 ->128 0.13829
117 ->129 -0.11672
119 ->125 0.13707

Excited State 21: Singlet 4.6325 eV 267.64 nm f=0.1099
115 ->121 0.43013
116 ->122 -0.21427
117 ->122 0.15026
119 ->124 0.14079
119 ->125 0.28050

Excited State 22: Singlet 4.6566 eV 266.26 nm f=0.0100
109 ->120 0.14344
111 ->120 -0.10336
112 ->120 -0.30323
113 ->120 -0.16653
115 ->121 0.33070
116 ->124 0.15062
116 ->128 0.12352
116 ->129 -0.11054
117 ->124 0.22484
117 ->125 -0.14534
117 ->128 0.16758
117 ->129 -0.13176

Excited State 23: Singlet 4.6796 eV 264.95 nm f=0.0096
111 ->120 -0.21274

112 ->120 0.24957
113 ->121 -0.10276
114 ->120 0.11714
115 ->122 0.10491
116 ->122 -0.25668
117 ->122 0.15453
117 ->124 0.15129
118 ->124 0.28208
118 ->128 0.13746
119 ->125 -0.11289

Excited State 24: Singlet 4.7264 eV 262.32 nm f=0.0040
109 ->120 -0.24532
111 ->120 0.33988
112 ->121 0.17733
113 ->121 -0.28700
114 ->120 -0.12373
114 ->121 -0.16241
116 ->122 0.16203
117 ->122 -0.12520
118 ->124 0.15853
118 ->125 -0.12105

Excited State 25: Singlet 4.7634 eV 260.28 nm f=0.0389
112 ->120 -0.13161
113 ->121 0.23464
114 ->120 0.13255
114 ->121 0.29697
115 ->122 -0.14811
116 ->122 0.11390
116 ->124 -0.11510
118 ->124 0.29209
118 ->125 -0.13194
118 ->128 0.13539
118 ->129 -0.13855

Excited State 26: Singlet 4.8372 eV 256.31 nm f=0.0074
109 ->120 0.40597
109 ->121 -0.10136
110 ->120 -0.30856
110 ->121 0.14518
111 ->120 0.10572
112 ->120 0.19760
113 ->120 0.10591
114 ->120 -0.18203
118 ->123 0.16826
118 ->124 0.15800

Excited State 27: Singlet 4.8771 eV 254.21 nm f=0.0039
112 ->121 0.16524
113 ->121 0.12448
114 ->121 0.13886
115 ->121 0.12875
118 ->124 -0.12517
119 ->124 0.14640
119 ->125 -0.27586
119 ->127 0.35337
119 ->128 -0.27894
119 ->129 0.20487

Excited State 28: Singlet 4.8908 eV 253.50 nm f=0.0093
109 ->120 -0.19685

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110 ->121	0.12802
111 ->120	-0.12108
111 ->121	0.10796
114 ->120	0.10650
118 ->123	0.55130

Excited State 29: Singlet 4.9094 eV 252.54 nm f=0.0568

109 ->120	-0.12087
110 ->120	-0.13076
110 ->121	0.10786
111 ->121	-0.23100
112 ->120	-0.12508
112 ->121	0.11995
114 ->121	0.14393
115 ->122	0.32172
118 ->123	0.15864
118 ->125	-0.21831
119 ->124	-0.14332
119 ->125	-0.11006
119 ->126	-0.16855

Excited State 30: Singlet 4.9504 eV 250.45 nm f=0.0358

109 ->121	0.20110
110 ->120	-0.25446
111 ->121	-0.10630
112 ->121	-0.24049
113 ->121	-0.18411
118 ->123	-0.12857
119 ->126	0.44273
119 ->127	0.11755

Excited State 31: Singlet 4.9881 eV 248.56 nm f=0.0672

109 ->120	-0.11129
109 ->121	-0.23689
111 ->121	0.40571
113 ->121	0.20578
114 ->121	-0.12961
114 ->122	0.10478
118 ->124	-0.14980
118 ->125	-0.19344
119 ->126	0.14475

Excited State 32: Singlet 5.0079 eV 247.58 nm f=0.0172

109 ->120	0.23542
110 ->120	0.43301
110 ->121	-0.10783
115 ->122	0.10696
118 ->123	0.25153
118 ->125	-0.14240
119 ->126	0.25399

Excited State 33: Singlet 5.0304 eV 246.47 nm f=0.0016

109 ->120	-0.10979
109 ->121	-0.16410
110 ->121	0.12580
111 ->121	-0.14570
112 ->121	0.30842
113 ->122	-0.11147
118 ->125	0.16611
119 ->125	0.14459
119 ->126	0.26903
119 ->127	0.19691

119 ->128 0.22199
119 ->129 -0.14751

Excited State 34: Singlet 5.0467 eV 245.67 nm f=0.0189
109 ->120 0.11339
111 ->122 0.24667
112 ->122 0.16787
113 ->122 -0.28405
114 ->122 0.49748

Excited State 35: Singlet 5.0772 eV 244.20 nm f=0.1547
109 ->121 0.22771
110 ->121 -0.11593
111 ->121 0.16211
112 ->121 -0.10197
119 ->126 -0.15726
119 ->127 0.45173
119 ->128 0.23881

Excited State 36: Singlet 5.1118 eV 242.54 nm f=0.0382
110 ->120 0.15759
110 ->121 0.15736
113 ->122 0.11738
116 ->123 0.23587
117 ->123 0.55019
118 ->123 -0.11331

Excited State 37: Singlet 5.1380 eV 241.30 nm f=0.0332
108 ->120 0.10309
109 ->121 -0.12981
112 ->121 -0.13710
113 ->122 -0.43560
114 ->122 -0.24303
115 ->122 0.29250
117 ->123 0.15060

Excited State 38: Singlet 5.1707 eV 239.78 nm f=0.0750
109 ->121 0.37020
110 ->121 -0.21130
112 ->121 0.31843
113 ->121 0.15523
113 ->122 -0.16500
117 ->123 0.14857
119 ->126 0.11372
119 ->127 -0.12717
119 ->128 -0.11150

Excited State 39: Singlet 5.2108 eV 237.94 nm f=0.0174
109 ->121 -0.11294
110 ->120 -0.14012
110 ->121 -0.33666
113 ->122 0.16301
114 ->123 0.15862
116 ->123 0.12112
116 ->125 0.11509
117 ->124 0.29451
117 ->125 0.18415
118 ->125 0.18994

Excited State 40: Singlet 5.2374 eV 236.73 nm f=0.1106
108 ->120 0.12049
109 ->122 0.10086

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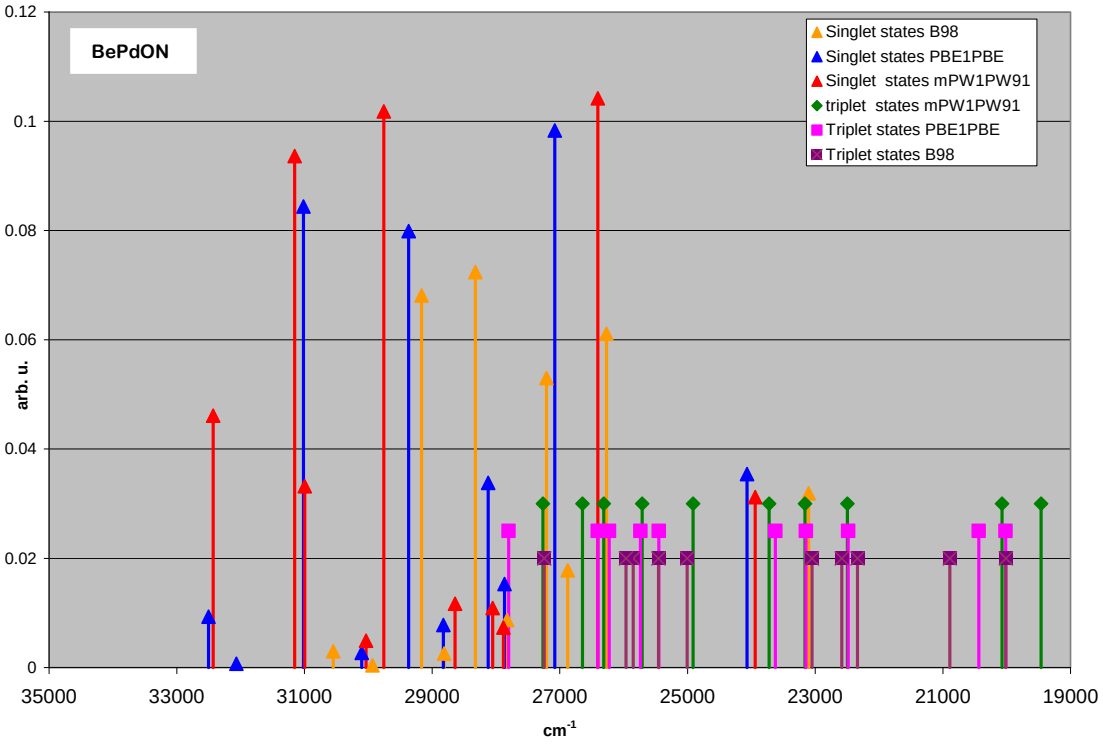
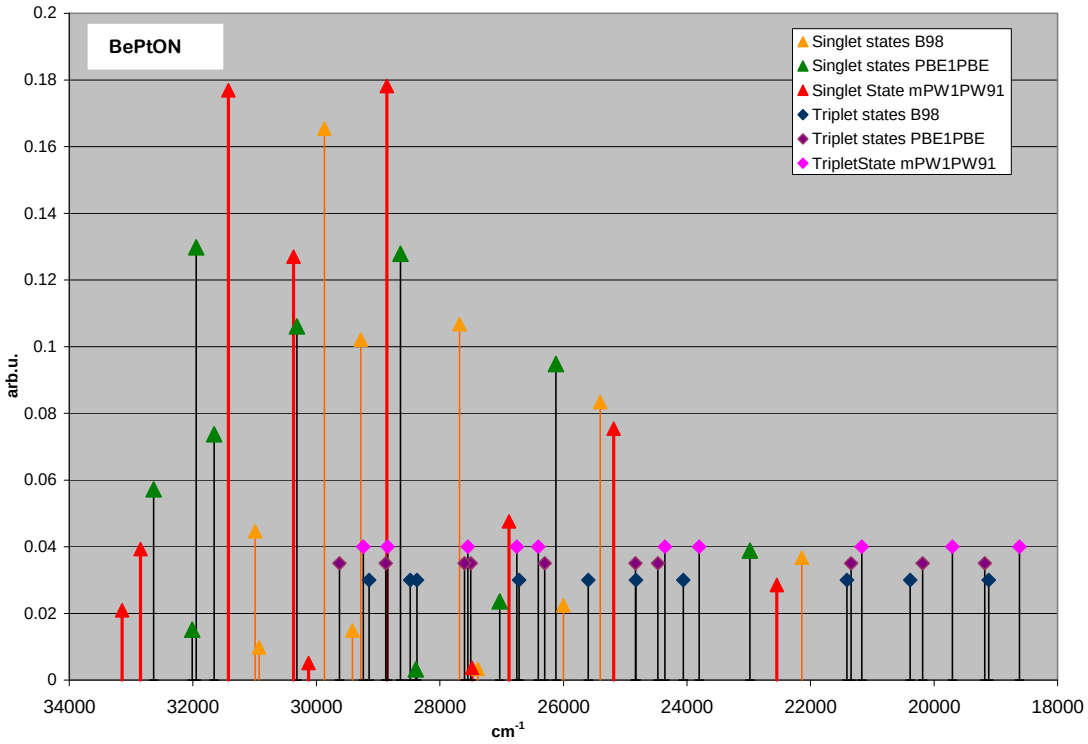
110 ->121	-0.14745
112 ->122	-0.19095
113 ->122	0.16054
113 ->124	-0.12409
113 ->128	-0.11269
113 ->129	0.10995
114 ->122	0.14949
115 ->122	0.16012
116 ->124	0.10287
116 ->125	-0.13498
117 ->124	-0.14142
118 ->124	0.20366
118 ->125	0.11791
119 ->129	0.12758

SI-12. Comparison between the first 10 transitions (singlet and triplet) in case of BEMON computed with different xc functionals (mPW1PW91,B98,PBE1PBE)





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