Supporting Information for:

Mechanism of the photochemical process by which phenalenone produces singlet molecular oxygen

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S1. Eigenvalues (in Hartrees) and eigenvectors of the diagonalization of the MS-CASPT2 effective hamiltonian matrix for the first five ^{1}A' states of the PN at the ground state geometry, averaging 5, 6 and 7 states at the reference Hamiltonian. An ANO-L basis set was used.

5 states averaged

State		GS	^{1}A’	^{1}A’	^{1}A’	^{1}A’
Eigenvalues		-573.93820	-573.81020	-573.79131	-573.76223	-573.74126
				Eigenvectors		
^{1}A’	GS	0.9948	-0.0986	-0.0022	-0.0164	-0.0157
^{1}A’	2 ^{1}(π-π*)	-0.0122	-0.1582	0.9799	0.1135	-0.0390
^{1}A’	3 ^{1}(π-π*)	-0.0811	-0.6432	-0.0509	-0.6173	-0.4426
^{1}A’	4 ^{1}(π-π*)	-0.0577	-0.7304	-0.1436	0.3988	0.5322
^{1}A’	5 ^{1}(π-π*)	0.0138	0.1337	0.1279	-0.6682	0.7203

6 states averaged

State		GS	^{1}A’	^{1}A’	^{1}A’	^{1}A’
Eigenvalues		-573.93826	-573.81091	-573.79116	-573.76214	-573.74558
				Eigenvectors		
^{1}A’	GS	-0.9944	-0.1023	-0.0023	-0.0122	-0.0204
^{1}A’	2 ^{1}(π-π*)	0.0111	-0.1431	0.9834	0.1037	-0.0188
^{1}A’	3 ^{1}(π-π*)	-0.0788	0.6283	0.0443	0.6047	0.4285
^{1}A’	4 ^{1}(π-π*)	-0.0625	0.7378	0.1286	-0.3450	-0.5399
^{1}A’	5 ^{1}(π-π*)	-0.0123	0.1383	0.1194	-0.6933	0.5312
^{1}A’	6 ^{1}(π-π*)	0.0274	-0.1033	-0.0111	0.1533	-0.4917

7 states averaged

State		GS	^{1}A’	^{1}A’	^{1}A’	^{1}A’
Eigenvalues		-573.93828	-573.81208		-573.76200	-573.74597

				-573.79121		
				Eigenvectors		
$^1A'$	GS	-0.9944	-0.1021	0.0004	-0.0110	0.0203
$^1A'$	2 $^1(\pi-\pi^*)$	0.0108	-0.1219	-0.9860	0.1004	0.0230
$^1A'$	3 $^1(\pi-\pi^*)$	-0.0781	0.6244	-0.0324	0.6047	-0.4211
$^1A'$	4 $^1(\pi-\pi^*)$	-0.0625	0.7352	-0.1051	-0.3318	0.5522
$^1A'$	5 $^1(\pi-\pi^*)$	-0.0136	0.1517	-0.1190	-0.6954	-0.5016
$^1A'$	6 $^1(\pi-\pi^*)$	-0.0286	0.1072	-0.0089	-0.1731	-0.5093
$^1A'$	7 $^1(\pi-\pi^*)$	-0.0027	0.0982	-0.0364	0.0159	-0.0757

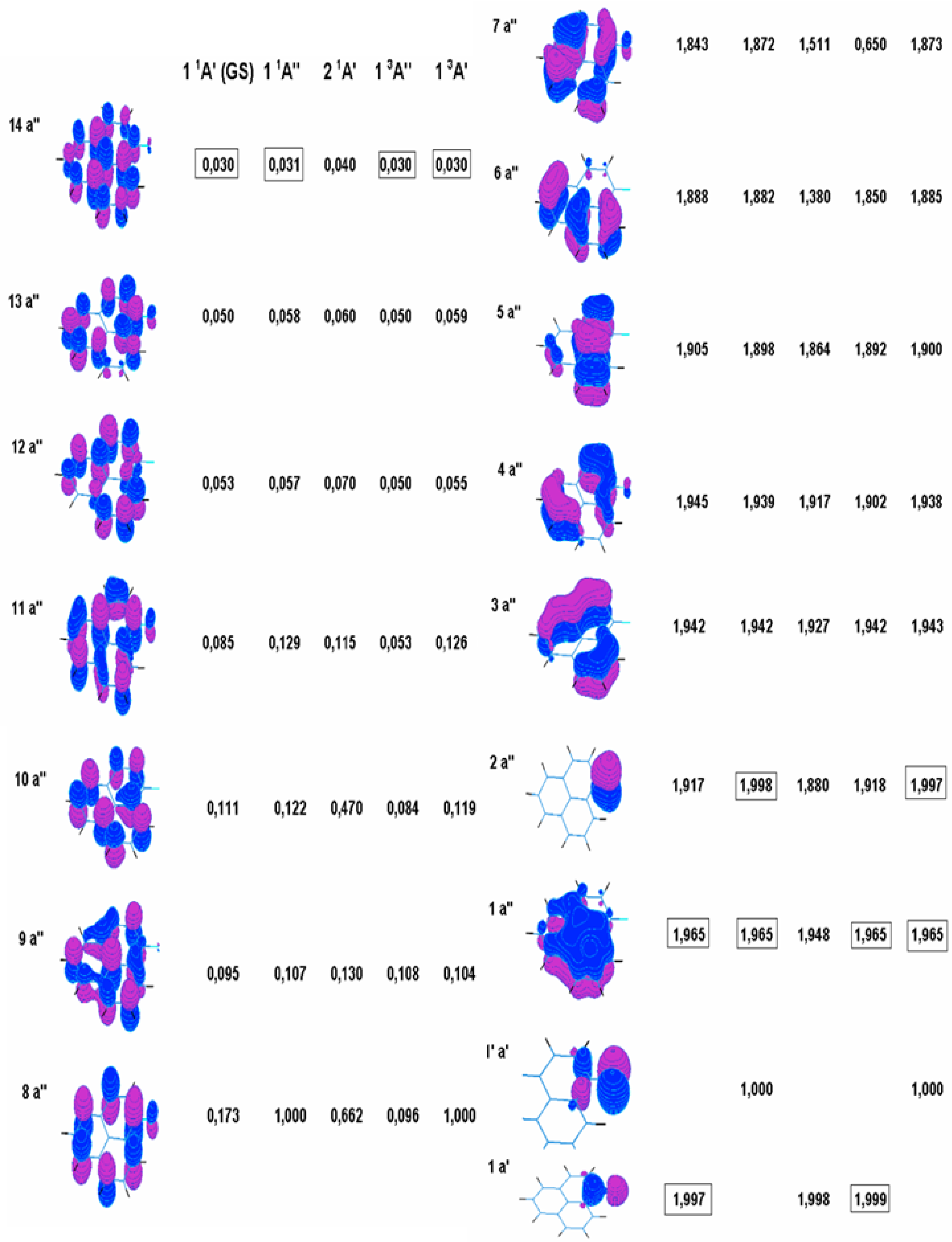
S2. Vertical excitations energies (in eV) at ground state equilibrium geometry calculated at the CASSCF(16,15) and MS-CASPT2 levels using a 6-31G plus polaritzation basis set. The state with the largest oscillator strength is shown in bold.

State	CASSCF	MS-CASPT2
$1^1A'$(GS)		
$2^1A'$	**3.97**	**3.57**
$3^1A'$	4.94	4.07
$4^1A'$	5.34	4.92
$5^1A'$	5.67	5.27
$6^1A'$	5.78	5.88
$7^1A'$	6.48	6.30
$8^1A'$	6.72	6.51
$1^1A''$	3.09	3.29
$2^1A'$	5.55	5.60
$1^3A'$	2.17	2.37
$1^3A''$	2.93	3.05

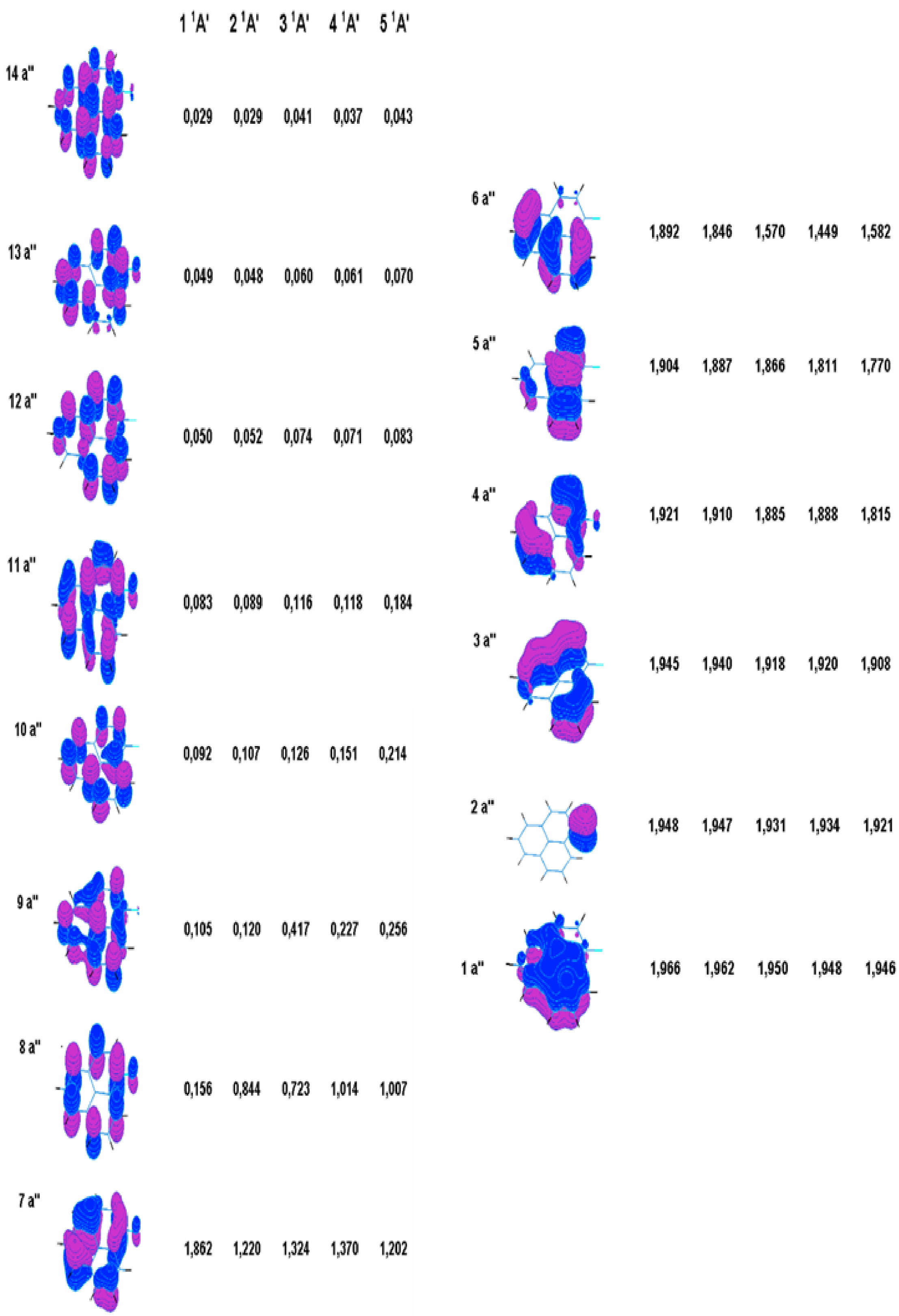
S3. Eigenvectors of the MS-CASPT2 effective hamiltonian matrix at the ground state geometry obtained at the CASSCF(16,15)/MS-CASPT2/6-31G* level.

State	$1^1A'$ (GS)	$2^1A'$	$3^1A'$	$4^1A'$
		eigenvector		
$1^1A'$ (GS)	0.996	-0.083	-0.005	0.003
$2^1A'$	-0.009	-0.157	0.984	0.068
$3^1A'$	-0.053	-0.538	-0.065	-0.627
$4^1A'$	0.062	0.771	0.130	-0.286
$5^1A'$	-0.013	-0.116	-0.093	0.664
$6^1A'$	-0.034	-0.136	-0.030	0.279
$7^1A'$	-0.002	-0.091	-0.033	-0.004
$8^1A'$	-0.009	0.213	0.007	0.045

S4. Natural orbital and occupancies for the ground state and for the $1^1A''$, $2^1A'$, $1^3A''$ and $^3A''$ excited states obtained at the CASSCF(16,15)/6-31G* level at the FC geometry. Marked orbitals are eliminated from the active space in the CASSCF(12,12) calculations.

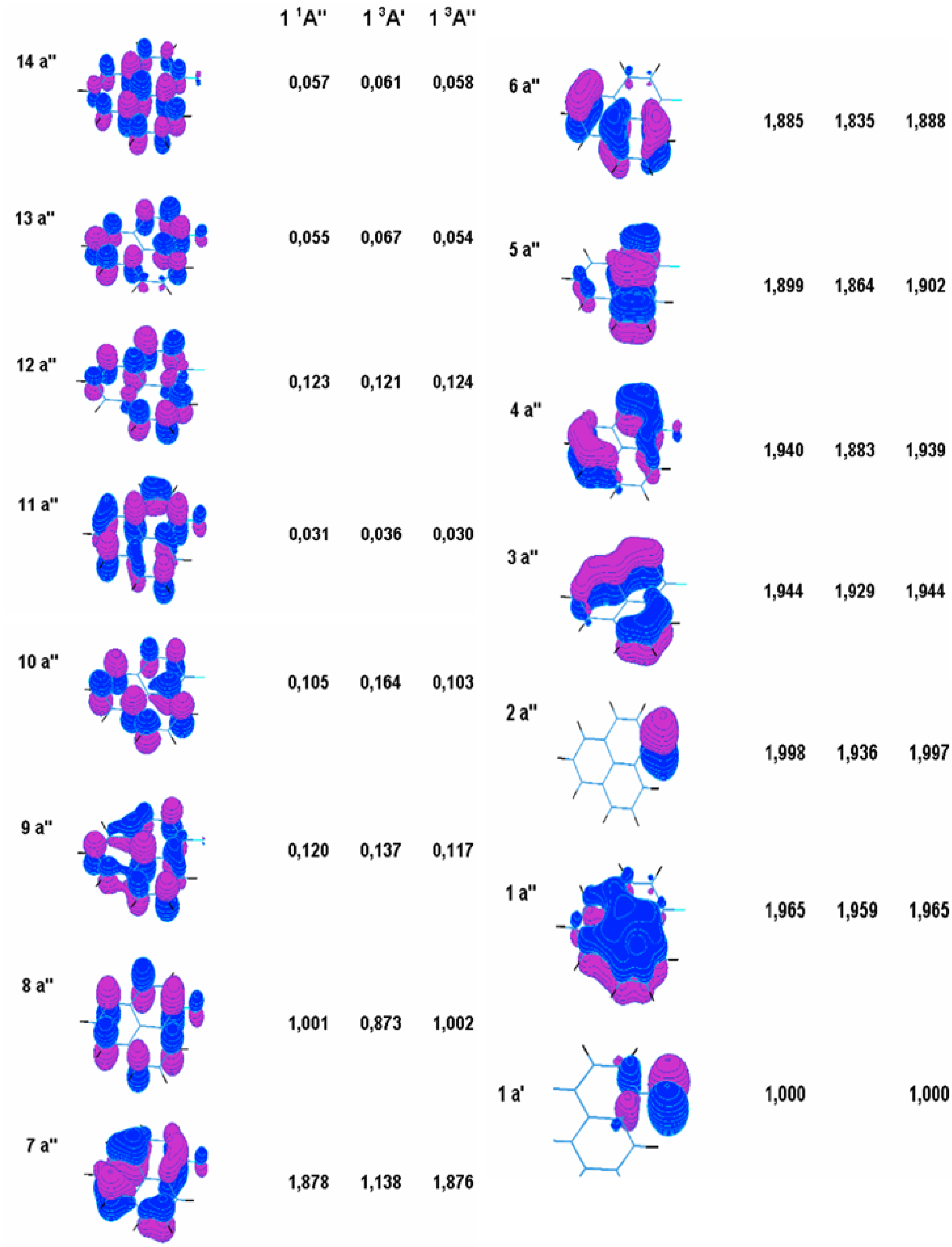


S5. Natural orbital and occupancies of the first five singlet states of A' symmetry, obtained at the CASSCF(16,15)/ANO-L level at the FC geometry.

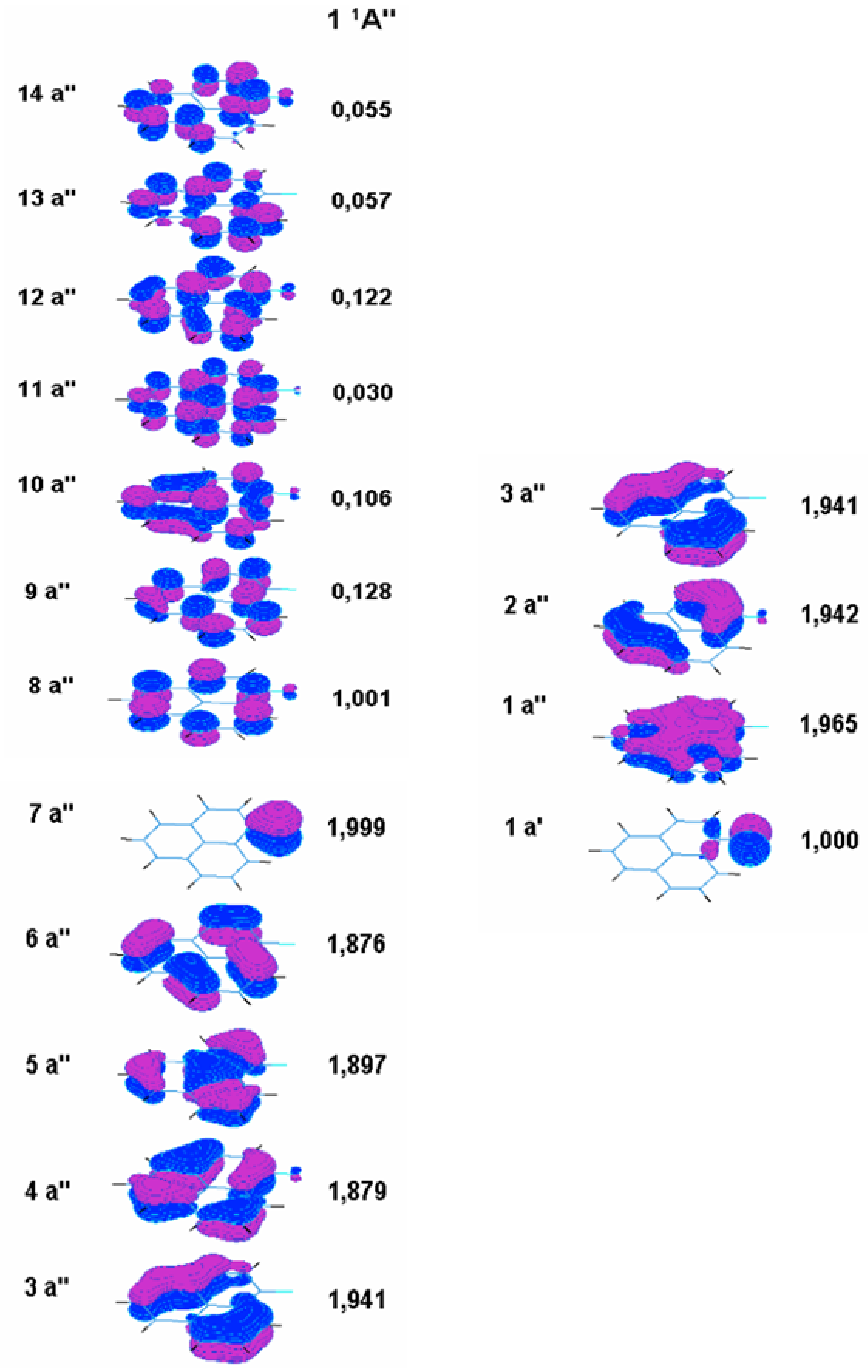


	$1\,^1A'$	$2\,^1A'$	$3\,^1A'$	$4\,^1A'$	$5\,^1A'$
14 a"	0,029	0,029	0,041	0,037	0,043
13 a"	0,049	0,048	0,060	0,061	0,070
12 a"	0,050	0,052	0,074	0,071	0,083
11 a"	0,083	0,089	0,116	0,118	0,184
10 a"	0,092	0,107	0,126	0,151	0,214
9 a"	0,105	0,120	0,417	0,227	0,256
8 a"	0,156	0,844	0,723	1,014	1,007
7 a"	1,862	1,220	1,324	1,370	1,202
6 a"	1,892	1,846	1,570	1,449	1,582
5 a"	1,904	1,887	1,866	1,811	1,770
4 a"	1,921	1,910	1,885	1,888	1,815
3 a"	1,945	1,940	1,918	1,920	1,908
2 a"	1,948	1,947	1,931	1,934	1,921
1 a"	1,966	1,962	1,950	1,948	1,946

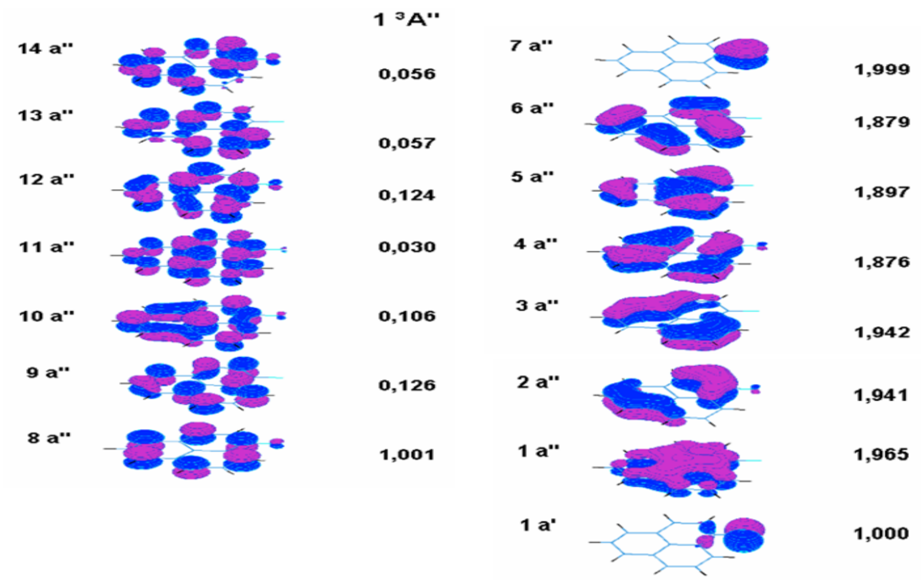
S6. Natural orbital and occupancies of the ^{1}A", ^{3}A" and ^{3}A" states obtained at CASSCF(16,15)/ANO-L level at the FC geometry.



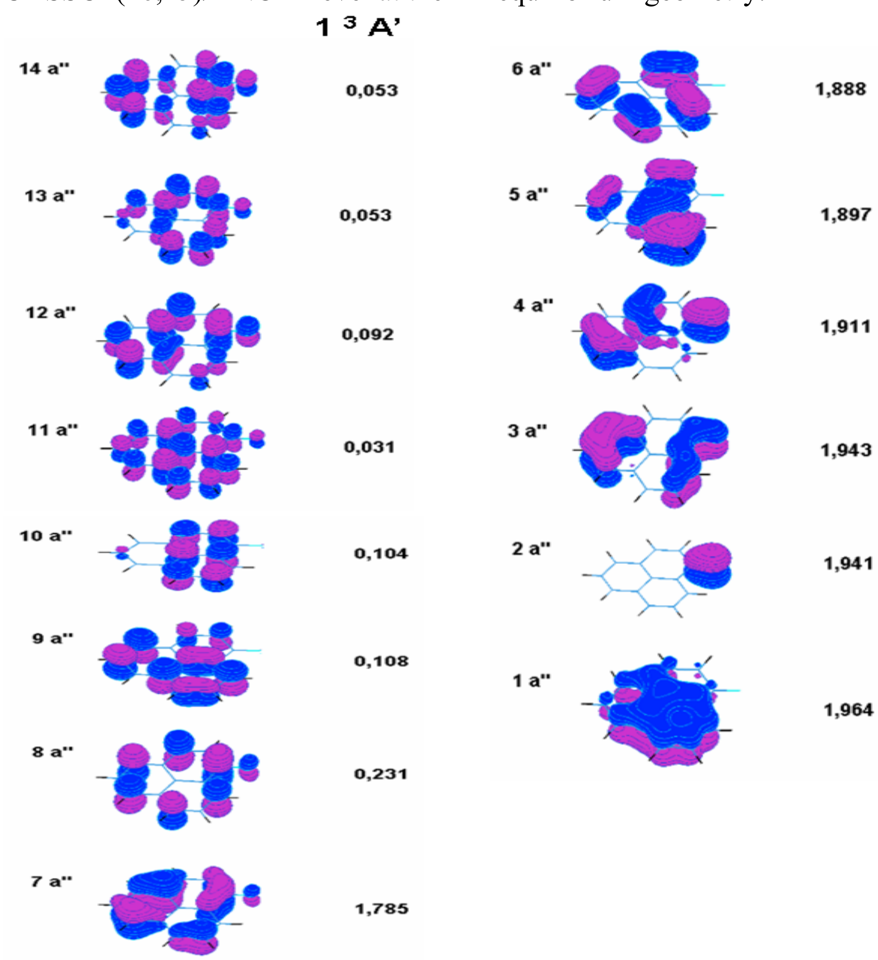
S7. Natural orbital and occupancies of the first excited singlet A" state obtained at the CASSCF(16,15)/ANO-L level at the ^{1}A" equilibrium geometry.



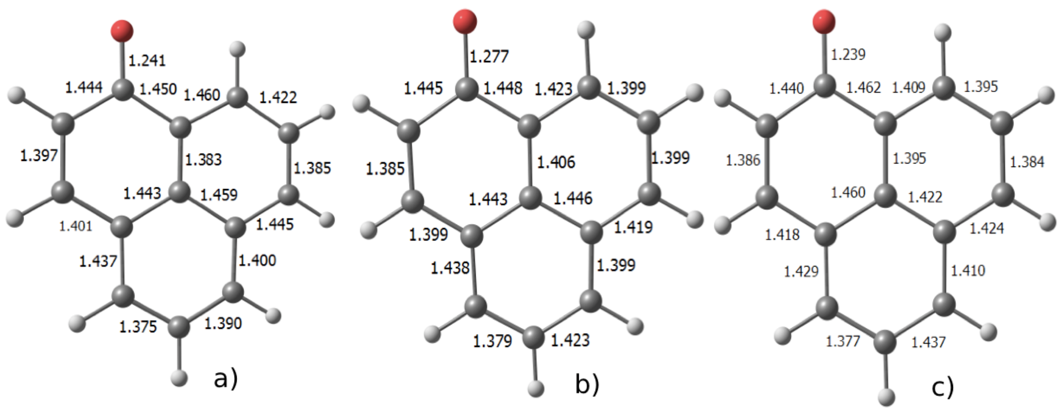
S8. Natural orbital and occupancies of the first excited triplet A'' state obtained at the CASSCF(16,15)/ANO-L level at the ^{3}A'' equilibrium geometry.



S9. Natural orbital and occupancies of the first excited triplet A' state obtained at the CASSCF(16,15)/ANO-L level at the ^{3}A' equilibrium geometry.



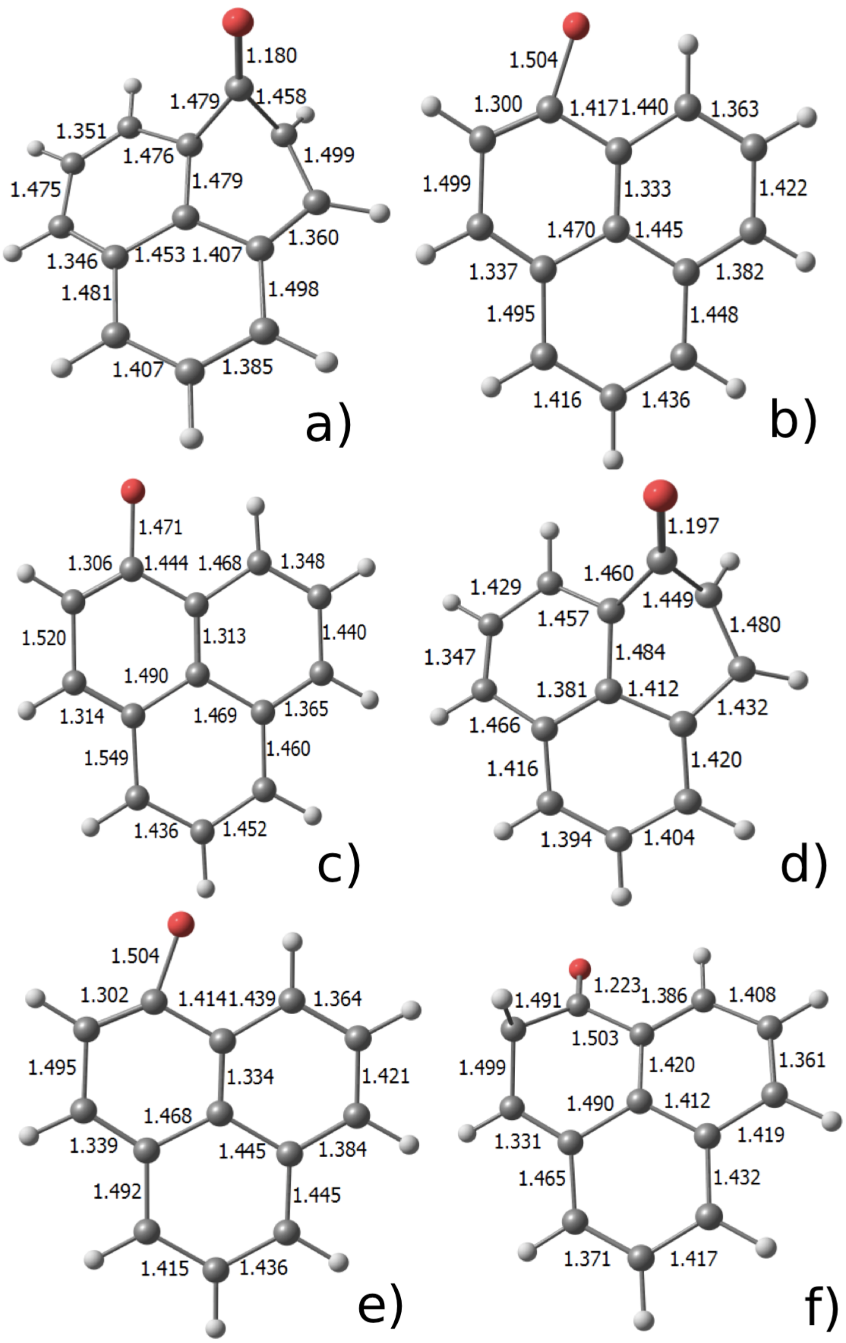
S10. a) Optimized geometry calculated at MS-CASPT2(16,15) level of the $^{1}(\pi\text{-}\pi^*)$ minumum. Optimized geometry calculated at CASSCF(16,15) level of the b)$^{1}(\pi\text{-}\pi^*)$-r3 and c) $^{1}(\pi\text{-}\pi^*)$-r4 minima.



S11. Vertical energies of four excited states at $^{1}(\pi\text{-}\pi^*)$, $^{1}(\pi\text{-}\pi^*)$-4r and $^{1}(\pi\text{-}\pi^*)$-3r calculed at MS-CASPT2(16,15)/ANO-L level relative to ground state minimum.

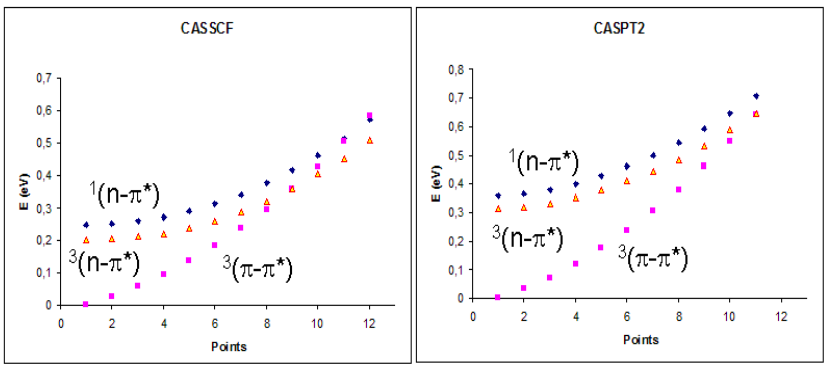
	$^{1}(\pi\text{-}\pi^*)$	$^{1}(\pi\text{-}\pi^*)$-4r	$^{1}(\pi\text{-}\pi^*)$-3r
$^{1}(\pi\text{-}\pi^*)$	2.97	3.13	3.06
^{1}(n-π^*)	2.93	3.15	3.11
^{3}(n-π^*)	2.88		
$^{3}(\pi\text{-}\pi^*)$	2.14		

S12. Geometries of S_0/S_1 conical intersections and $S_0/\ T_1$ ISC. a) $S_0/^1(\pi\text{-}\pi^*)$ non-planar CI ; b) $S_0/^1(n\text{-}\pi^*)$ planar CI; c) $S_0/^3(\pi\text{-}\pi^*)$ non-planar ISC; d) $S_0/^3(\ \pi\text{-}\pi^*)$ planar ISC; e) $S_0/^3(n\text{-}\pi^*)$ non-planar ISC; f) $S_0/^3(n\text{-}\pi^*)$ planar ISC.



S13. Energies (in eV) and energetic profiles of the PES of the ^{1}(n-π*), ^{3}(π-π*) and ^{3}(n-π*) states from the ^{1}(n-π*) minimun to the STC ^{1}(n-π*)/^{3}(π-π*). The profiles are obtained with linear geometric linear interpolations at CASSCF(12,12)/CASPT2/6-31G(d) level.

		ΔE CASSCF 1^1A''	ΔE CASSCF 1^3A'	ΔE CASSCF 1^3A''	ΔE CASPT2 1^1A''	ΔE CASPT2 1^3A'	ΔE CASPT2 1^3A''
1^1A''	1	0,22	0,00	0,18	0,36	0,00	0,31
	2	0,23	0,03	0,21	0,36	0,03	0,32
	3	0,25	0,07	0,22	0,38	0,07	0,33
	4	0,26	0,11	0,24	0,40	0,12	0,35
	5	0,29	0,16	0,26	0,43	0,17	0,38
	6	0,32	0,21	0,29	0,46	0,24	0,41
	7	0,35	0,27	0,32	0,50	0,30	0,44
	8	0,39	0,33	0,36	0,54	0,38	0,49
	9	0,44	0,40	0,40	0,59	0,46	0,53
	10	0,49	0,48	0,45	0,65	0,55	0,59
STC	11	0,55	0,56	0,51	0,71	0,64	0,65



S14. Absorption energies (in eV), oscillator strengths (f), dipole moments (μ in Debyes) and weight of the CASSCF reference in the CASPT2 wavefunction (Weight) for PN computed with ANO-L basis set and an active space of 16 electrons and 15 orbitals.

Symm	State	CASSCF	SS-CASPT2	Weight	μ	f	MS-CASPT2	μ	f
^{1}A'	GS	0.00	0.00	0.6336	3.5		0.00	4.1	
^{1}A''	1 ^{1}(n-π*)	3.22	3.32	0.6326	0.8	$<10^{-3}$	3.36	0.8	$<10^{-3}$
^{1}A'	2 ^{1}(π-π*)	3.94	3.96	0.6323	3.8	0.0100	3.48	6.63	0.2012
^{1}A'	3 ^{1}(π-π*)	4.89	4.29	0.6257	4.8	0.0779	4.00	3.95	0.0180

^{1}A'	4 ^{1}(π-π*)	5.27	4.18	0.6219	5.7	0.1801	4.79	3.59	0.0163
^{1}A'	5 ^{1}(π-π*)	5.60	5.01	0.6263	4.0	0.0208	5.36	3.64	<10^{-3}
^{3}A'	^{3}(π-π*)	2.33	2.53	0.6344	3.4	<10^{-3}	2.57	3.4	<10^{-3}
^{3}A''	^{3}(n-π*)	3.09	3.20	0.6344	0.7	<10^{-3}	3.24	0.7	<10^{-3}

S15. Cartesian coordinates in Angstroms for the minima of low-lying PES and optimized crossing points.

GS

O	0.089057	-3.350957	0.000000
C	0.865441	1.406232	0.000000
C	2.271274	1.195375	0.000000
C	2.791838	-0.079625	0.000000
C	1.931532	-1.200109	0.000000
C	0.559896	-1.030186	0.000000
C	0.004465	0.284082	0.000000
C	-0.342027	-2.214734	0.000000
C	-1.415669	0.479212	0.000000
C	-1.926556	1.760776	0.000000
C	-1.064324	2.887739	0.000000
C	0.297527	2.716421	0.000000
C	-1.793086	-1.953482	0.000000
C	-2.284433	-0.697333	0.000000
H	2.926388	2.048439	0.000000
H	3.856217	-0.228381	0.000000
H	2.334561	-2.194654	0.000000
H	-2.433769	-2.815495	0.000000
H	-3.347735	-0.534001	0.000000
H	-2.991793	1.910003	0.000000
H	-1.486360	3.876119	0.000000
H	0.953336	3.568719	0.000000

^{1}(n-π*)

O	0.135034	-3.390901	0.000000
C	0.858540	1.403220	0.000000
C	2.259977	1.186510	0.000000
C	2.783502	-0.104646	0.000000
C	1.942758	-1.214201	0.000000
C	0.533836	-1.040968	0.000000
C	-0.017013	0.274466	0.000000

C	-0.368861	-2.133937	0.000000
C	-1.431052	0.469034	0.000000
C	-1.944098	1.794315	0.000000
C	-1.085345	2.887946	0.000000
C	0.297600	2.705131	0.000000
C	-1.745609	-1.956315	0.000000
C	-2.274209	-0.665654	0.000000
H	2.920024	2.035201	0.000000
H	3.848923	-0.247346	0.000000
H	2.358390	-2.204221	0.000000
H	-2.390872	-2.815061	0.000000
H	-3.340457	-0.531420	0.000000
H	-3.009034	1.942493	0.000000
H	-1.490233	3.883850	0.000000
H	0.953985	3.556667	0.000000

$^1(\pi\text{-}\pi^*)$

O	0.166339	-3.367944	0.000000
C	0.870331	1.409692	0.000000
C	2.272115	1.191821	0.000000
C	2.794092	-0.106319	0.000000
C	1.945478	-1.218214	0.000000
C	0.534959	-1.030840	0.000000
C	-0.011397	0.264162	0.000000
C	-0.331023	-2.191921	0.000000
C	-1.440431	0.465467	0.000000
C	-1.962578	1.805384	0.000000
C	-1.108085	2.887340	0.000000
C	0.300616	2.687314	0.000000
C	-1.754509	-1.946190	0.000000
C	-2.270387	-0.660467	0.000000
H	2.940521	2.051015	0.000000
H	3.871729	-0.247664	0.000000
H	2.320335	-2.236960	0.000000
H	-2.407555	-2.814908	0.000000
H	-3.350400	-0.514890	0.000000
H	-3.040634	1.951771	0.000000
H	-1.501150	3.900012	0.000000
H	0.957415	3.556500	0.000000

$^1(\pi\text{-}\pi^*)$-r3

O	0.094783	-3.363466	0.000000
C	0.854254	1.405225	0.000000
C	2.284567	1.201292	0.000000
C	2.813753	-0.078595	0.000000
C	1.972702	-1.225815	0.000000
C	0.523910	-1.045151	0.000000

C	-0.010938	0.230633	0.000000
C	-0.347785	-2.204397	0.000000
C	-1.436417	0.457254	0.000000
C	-1.940129	1.802648	0.000000
C	-1.092684	2.886062	0.000000
C	0.282312	2.683059	0.000000
C	-1.769713	-1.950579	0.000000
C	-2.290117	-0.653687	0.000000
H	2.932242	2.059021	0.000000
H	3.880574	-0.209053	0.000000
H	2.375969	-2.216637	0.000000
H	-2.420599	-2.804588	0.000000
H	-3.355551	-0.507039	0.000000
H	-3.005415	1.947634	0.000000
H	-1.488187	3.884342	0.000000
H	0.938253	3.535997	0.000000

^{1}(π-π*)-r4

O	0.127574	-3.350491	0.000000
C	0.868612	1.386873	0.000000
C	2.279099	1.192103	0.000000
C	2.791965	-0.093584	0.000000
C	1.939661	-1.198439	0.000000
C	0.540510	-1.030261	0.000000
C	0.003987	0.257415	0.000000
C	-0.335519	-2.200929	0.000000
C	-1.440623	0.470888	0.000000
C	-1.963374	1.800413	0.000000
C	-1.107502	2.879498	0.000000
C	0.316363	2.683840	0.000000
C	-1.752154	-1.945045	0.000000
C	-2.287767	-0.666592	0.000000
H	2.928507	2.048058	0.000000
H	3.856640	-0.242175	0.000000
H	2.331729	-2.195649	0.000000
H	-2.397008	-2.804330	0.000000
H	-3.352153	-0.520948	0.000000
H	-3.026971	1.943693	0.000000
H	-1.492717	3.881986	0.000000
H	0.966925	3.537838	0.000000

CI ^{3}(π-π*)/^{3}(n-π*)

O	0.284054	-3.316971	0.000000
C	0.853134	1.391101	0.000000
C	2.262467	1.171335	0.000000
C	2.774668	-0.096224	0.000000
C	1.904283	-1.220072	0.000000

C	0.541837	-1.036405	0.000000
C	-0.020362	0.286273	0.000000
C	-0.413361	-2.110988	0.000000
C	-1.439619	0.491566	0.000000
C	-1.933876	1.767842	0.000000
C	-1.053537	2.893295	0.000000
C	0.295889	2.709796	0.000000
C	-1.780136	-1.965669	0.000000
C	-2.294904	-0.690604	0.000000
H	2.921008	2.021652	0.000000
H	3.837261	-0.256313	0.000000
H	2.354536	-2.202134	0.000000
H	-2.436581	-2.816034	0.000000
H	-3.360419	-0.556803	0.000000
H	-2.997437	1.931002	0.000000
H	-1.467386	3.885610	0.000000
H	0.964262	3.552905	0.000000

ISC ^{1}(n-π*)/^{3}(π-π*)

O	0.284054	-3.316971	0.000000
C	0.853134	1.391101	0.000000
C	2.262467	1.171335	0.000000
C	2.774668	-0.096224	0.000000
C	1.904283	-1.220072	0.000000
C	0.541837	-1.036405	0.000000
C	-0.020362	0.286273	0.000000
C	-0.413361	-2.110988	0.000000
C	-1.439619	0.491566	0.000000
C	-1.933876	1.767842	0.000000
C	-1.053537	2.893295	0.000000
C	0.295889	2.709796	0.000000
C	-1.780136	-1.965669	0.000000
C	-2.294904	-0.690604	0.000000
H	2.921008	2.021652	0.000000
H	3.837261	-0.256313	0.000000
H	2.354536	-2.202134	0.000000
H	-2.436581	-2.816034	0.000000
H	-3.360419	-0.556803	0.000000
H	-2.997437	1.931002	0.000000
H	-1.467386	3.885610	0.000000
H	0.964262	3.552905	0.000000

CI ^{1}(n-π*)/SO

O	0.532069	-3.248091	0.000000
C	0.871709	1.385387	0.000000
C	2.231556	1.140047	0.000000
C	2.751428	-0.184045	0.000000

C	1.894087	-1.243129	0.000000
C	0.479257	-0.976987	0.000000
C	-0.029430	0.255172	0.000000
C	-0.413218	-2.077918	0.000000
C	-1.487093	0.442107	0.000000
C	-2.002787	1.845608	0.000000
C	-1.100132	2.936523	0.000000
C	0.320531	2.723864	0.000000
C	-1.712039	-2.018442	0.000000
C	-2.283162	-0.632270	0.000000
H	2.916602	1.969252	0.000000
H	3.814804	-0.337746	0.000000
H	2.282824	-2.250262	0.000000
H	-2.364629	-2.869976	0.000000
H	-3.353301	-0.532005	0.000000
H	-3.064519	2.003419	0.000000
H	-1.480325	3.941388	0.000000
H	0.991550	3.562264	0.000000

CI ^{1}(π-π*)/SO

O	-0.254942	-2.751409	1.872222
C	0.853521	1.396227	0.085021
C	2.154367	1.108423	-0.105979
C	2.587184	-0.277407	-0.368460
C	1.746321	-1.334293	-0.337084
C	0.337292	-1.120087	0.048144
C	-0.094036	0.294544	0.074146
C	-0.389373	-2.071455	0.917018
C	-1.486267	0.471591	-0.031941
C	-2.010378	1.871253	0.067316
C	-1.124013	2.925360	0.212712
C	0.272480	2.752824	0.204071
C	-1.168135	-1.877324	-0.300703
C	-2.107842	-0.709376	-0.295228
H	2.880053	1.903407	-0.124213
H	3.624654	-0.453438	-0.588424
H	2.111320	-2.330716	-0.509331
H	-1.315277	-2.697163	-0.984303
H	-3.159693	-0.839721	-0.454027
H	-3.068015	2.050750	0.047269
H	-1.521234	3.922497	0.299733
H	0.927794	3.599676	0.272163

ISC ^{3}(n-π*)/SO plane

O	0.534350	-3.244668	0.000000
C	0.871264	1.386953	0.000000
C	2.232798	1.139187	0.000000

C	2.750891	-0.183803	0.000000
C	1.891720	-1.243423	0.000000
C	0.478168	-0.975564	0.000000
C	-0.030523	0.257612	0.000000
C	-0.411138	-2.075314	0.000000
C	-1.486535	0.443534	0.000000
C	-2.001558	1.843895	0.000000
C	-1.099772	2.934449	0.000000
C	0.320701	2.722728	0.000000
C	-1.711927	-2.016154	0.000000
C	-2.282510	-0.633787	0.000000
H	2.918379	1.967925	0.000000
H	3.814145	-0.338410	0.000000
H	2.276549	-2.252528	0.000000
H	-2.363614	-2.868409	0.000000
H	-3.352622	-0.533503	0.000000
H	-3.063266	2.002241	0.000000
H	-1.480389	3.939167	0.000000
H	0.990674	3.562032	0.000000

ISC ^{3}(n-π*)/SO

O	-0.069413	-3.293834	0.888204
C	0.814244	1.323590	-0.165106
C	2.215634	1.102277	-0.210721
C	2.736622	-0.145736	-0.058680
C	1.890828	-1.248431	0.165485
C	0.515834	-1.075551	0.161613
C	-0.046468	0.210970	-0.047713
C	-0.401277	-2.252605	0.339763
C	-1.519941	0.422215	0.022521
C	-1.989112	1.798750	0.195178
C	-1.118491	2.852557	0.088363
C	0.262434	2.644764	-0.150894
C	-1.685585	-1.956184	-0.356373
C	-2.307814	-0.650526	0.039034
H	2.867788	1.947562	-0.343535
H	3.801405	-0.292039	-0.083699
H	2.297386	-2.227178	0.335473
H	-1.521003	-2.026525	-1.427599
H	-3.345840	-0.607718	0.314729
H	-3.037149	1.961230	0.366826
H	-1.486543	3.859263	0.170364
H	0.922244	3.487309	-0.243114

ISC ^{3}(π-π*)/SO plane

O	0.229035	-3.456189	0.000000
C	0.890236	1.389180	0.000000

C	2.238884	1.180647	0.000000
C	2.786424	-0.151720	0.000000
C	1.960409	-1.217533	0.000000
C	0.510122	-0.990241	0.000000
C	-0.000006	0.220112	0.000000
C	-0.388141	-2.121257	0.000000
C	-1.477368	0.414030	0.000000
C	-2.028268	1.861787	0.000000
C	-1.110266	2.965922	0.000000
C	0.323514	2.734267	0.000000
C	-1.690493	-2.022848	0.000000
C	-2.283648	-0.623385	0.000000
H	2.907939	2.023061	0.000000
H	3.853402	-0.283846	0.000000
H	2.328354	-2.222752	0.000000
H	-2.323911	-2.888982	0.000000
H	-3.353279	-0.518606	0.000000
H	-3.091518	1.999282	0.000000
H	-1.482984	3.973046	0.000000
H	0.997346	3.570185	0.000000

ISC $^3(\pi-\pi^*)$/SO

O	-0.219351	-2.819672	1.850813
C	0.795336	1.380926	0.150121
C	2.206240	1.067633	-0.098149
C	2.583129	-0.191289	-0.394277
C	1.683551	-1.301222	-0.351618
C	0.318910	-1.087546	0.110453
C	-0.103204	0.333018	0.188309
C	-0.382596	-2.067913	0.933959
C	-1.497910	0.514632	0.067869
C	-2.014020	1.837336	0.108971
C	-1.108476	2.906825	0.202247
C	0.268756	2.694751	0.192014
C	-1.166647	-1.858146	-0.265851
C	-2.126993	-0.731715	-0.250138
H	2.922431	1.869064	-0.112489
H	3.609577	-0.391731	-0.645547
H	2.049041	-2.297412	-0.511067
H	-1.288850	-2.667578	-0.967743
H	-3.115581	-0.826802	-0.654021
H	-3.070154	2.021115	0.029988
H	-1.485396	3.913191	0.230672
H	0.937987	3.536694	0.185603