Unveiling the Intersystem Crossing Dynamics in N-Annulated Perylene Bisimides

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Supplementary Information (SI)

Contents

Section 1: Materials and Methods

All chemicals were obtained from commercial suppliers and used as received without further purification. All reactions were carried out in oven-dried glassware and whenever required, were under dry nitrogen in dried, anhydrous solvents using standard gastight syringes, septa and cannulae. Solvents were dried and distilled by following the standard procedures. TLC analyses were conducted on aluminium plates coated with silica gel 60 F254 (0.25 mm, Merck), and short and long wavelength UV lamps TLC plates were used to observe TLC plates. Column chromatography was executed using silica gel of 200-400 mesh utilizing an appropriate solvent polarity correlated with the TLC mobility noticed for each particular molecule. Yields are recorded for chromatographically and spectroscopically homogenous substances. 500 MHz Bruker avance DPX spectrometer was used for recording ^{1}H and ^{13}C NMR spectra. 1,1,1,1-tetramethyl silane (TMS) was used as Internal standard for ^{1}H and ^{13}C NMR. High-resolution mass spectra (HRMS) were recorded on Thermo scientific Q exactive mass spectrometer utilizing the atmospheric pressure chemical ionization (APCI, positive mode) technique. Photophysical measurements of the compounds were performed in a cuvette of 3 mm path length. Absorption and emission spectra were recorded using Shimadzu UV-3600 UV-Vis-NIR and Horiba Jobin Yvon Fluorolog spectrometers, respectively.

1.1 Calculating the rate of Intersystem Crosssing (k_{ISC})

Rate of Intersystem Crossing (k_{ISC}) was calculated using triplet quantum yield (ϕ_T) and decay time constant of singlet ($\tau_{A\rightarrow B}$),[1]

$$k_{ISC} = \frac{\phi_T}{\tau_{A\rightarrow B}} \qquad (1)$$

Where $\tau_{A\rightarrow B}$ is the decay time constant of singlet excited state fitted from fsTA and ϕ_T is the triplet quantum yield.

1.2 Calculating the adiabatic energies

To describe the shapes of the potential energy surfaces, adiabatic energies were computed. The energy of the excited state with respect to the minimum energy $E_{S_0}(R(S_0))$, were calculated using the following equations.[2] More information can be taken from figure S9.

$$E_{adiab}^{S_0}(R(T_2)) = E_{S_0}(R(T_2)) - E_{S_0}(R(S_0))$$

$$E_{adiab}^{S_1}(R(T_2)) = E_{S_1}(R(T_2)) - E_{S_0}(R(S_0))$$

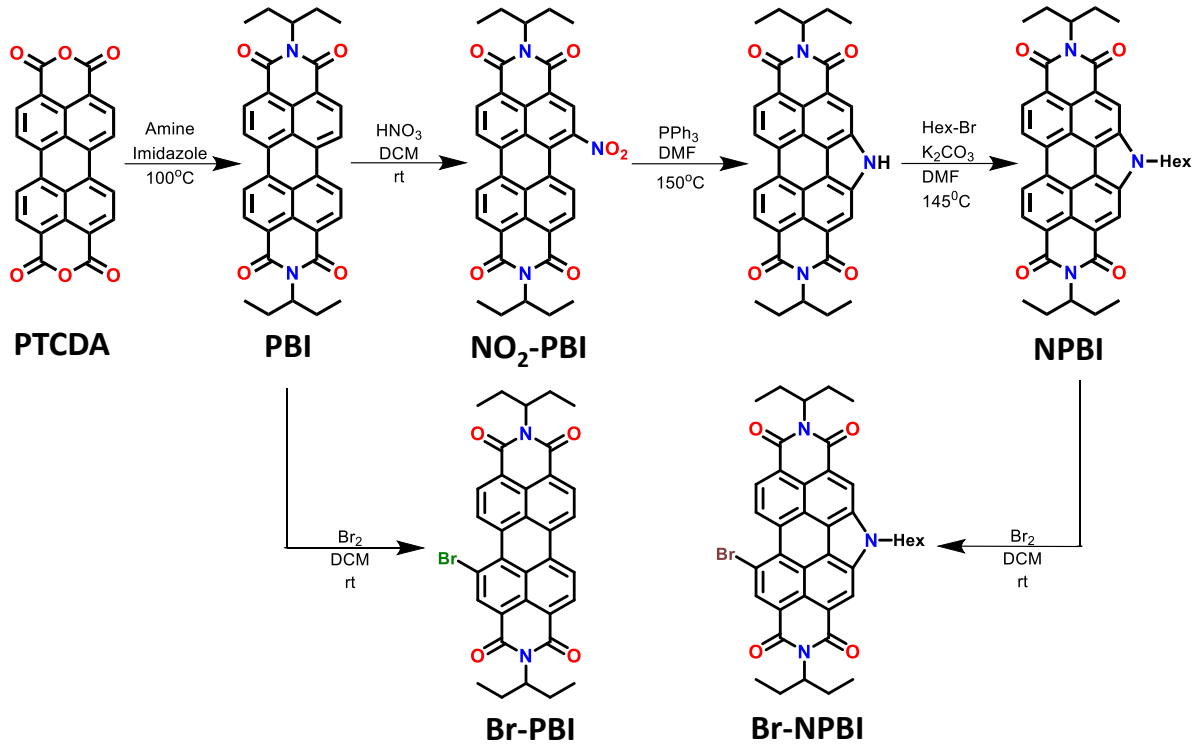
$$E_{adiab}^{T_2}(R(T_2)) = E_{T_1}(R(T_2)) - E_{S_0}(R(S_0))$$

$$E_{adiab}^{S_0}(R(S_1)) = E_{S_0}(R(S_1)) - E_{S_0}(R(S_0))$$

$$E_{adiab}^{S_1}(R(S_1)) = E_{S_1}(R(S_1)) - E_{S_0}(R(S_0))$$

$$E_{adiab}^{T_2}(R(S_1)) = E_{T_1}(R(S_1)) - E_{S_0}(R(S_0))$$

Section 2: Synthesis and Characterization



Scheme S1: Synthesis scheme for **PBI**, **NPBI**, **Br-PBI** and **Br-NPBI.**

Synthesis of Br-NPBI:

The compound was synthesized according to the previously reported procedure.[3,4] To a mixture of **NPBI** (0.44g, $9.2*10^{-4}$ mmol) in CH_2Cl_2 (25 mL), liquid Br_2 was added dropwise with stirring. The reaction mixture was covered with a Teflon cap and continued to stir for 2 hours at room temperature. Complete consumption of starting material indicated in TLC analysis confirms completion of the reaction. Unreacted bromine was quenched using air bubbling and the solvent was removed under reduced pressure. The crude product was purified by silica gel column chromatography using CH_2Cl_2 : Pet ether as eluent. Product concentrated using rotary evaporation was slurried in methanol and further filtration was carried out using Buchner funnel to yield dark red solid (Yield = 91%).

^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ = 10.21 (d, 1H), 9.00-8.98 (m, 3H), 8.83 (d, 1H), 5.23-5.10 (m, 2H), 4.84 (t, 2H), 2.35-2.24 (m, 4H), 2.14 (s, 2H), 1.96 (t, 4H), 1.38-1.24 (m, 10H), 1.23-0.92 (m, 12H)

^{13}C NMR (500 MHz, $CDCl_3$, ppm) δ = 134.36, 134.16, 132.12, 130.19, 127.33, 124.05, 123.46, 123.08, 121.95, 121.25, 118.58, 118.15, 58.07, 57.91, 46.82, 31.29, 26.82, 25.23, 25.17, 22.42, 13.88, 11.50

HRMS (APCI) *m/z* calculated for $C_{40}H_{40}BrN_3O_4$ $[(M+H)^+]$ =706.2275, found: 706.2254

Section 3: Tables

Table S1: Solvent dependent fluorescence quantum yield measurements of **Br-NPBI** and **NPBI**.

	Fluorescence Quantum Yield ($\Phi_f(\%)$)	
	Br-NPBI	NPBI [a]
Toluene	2.01	68
Acetone	2.38	61
Acetonitrile	2.12	62

[a] Fluorescence quantum yield was obtained from previously published results

Table S2: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0). The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2 for **PBI** at CAM-B3LYP/def2-SVP levels of theory. For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies.

PBI CAM-B3LYP/ def2-SVP	Energy relative to the ground state energy at R(S_0) in eV			
Geometry	S_0	S_1	T_1	T_2
R(S_0)	0	2.80	1.67	2.98
R(S_1)	0.19	2.60	1.40	2.97
R(T_2)	0.287	2.71	1.50	2.92

Table S3: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0). The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2 for **Br-PBI** at CAM-B3LYP/def2-SVP levels of theory. For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies.

Br-PBI CAMB3LYP/ def2-SVP	Energy relative to the ground state energy at R(S_0) in eV			
Geometry	S_0	S_1	T_1	T_2
R(S_0)	0	2.79	1.71	2.96
R(S_1)	0.21	2.57	1.43	2.94
R(T_2)	0.29	2.68	1.53	2.87

Table S4: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0). The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2 for **NPBI** at CAM-B3LYP/def2-SVP levels of theory. For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies.

NPBI CAM-B3LYP/ def2-SVP	Energy relative to the ground state energy at R(S_0) in eV			
Geometry	S_0	S_1	T_1	T_2
R(S_0)	0	2.91	1.87	2.71
R(S_1)	0.16	2.74	1.64	2.71
R(T_2)	0.12	2.84	1.76	2.61

Table S5: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0). The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2 for **Br-NPBI** at CAM-B3LYP/def2-SVP levels of theory. For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies

Br-NPBI CAMB3LYP/ def2-SVP	Energy relative to the ground state energy at R(S_0) in eV			
Geometry	S_0	S_1	T_1	T_2
R(S_0)	0	2.91	1.89	2.69
R(S_1)	0.16	2.74	1.67	2.68
R(T_2)	0.12	2.83	1.78	2.59

Table S6: Camparision of Singlet excited state computed using TD-DFT and TDA at CAM-B3LYP/aug-cc-pVDZ levels of theory**.**

S_1 Energy relative to ground state energy at R(S_0) (eV)	**PBI**		**Br-PBI**		**NPBI**		**Br-NPBI**	
	TD-DFT	**TDA**	**TD-DFT**	**TDA**	**TD-DFT**	**TDA**	**TD-DFT**	**TDA**
R(S_0)	2.70	3.01	2.72	2.99	2.82	3.10	2.83	3.09
R(S_1)	2.49	2.85	2.49	2.81	2.64	2.96	2.66	2.95
R(T_2)	2.61	2.96	2.60	2.92	2.74	3.04	2.74	3.02

Table S7: The computed spin-orbit coupling values for **PBI, Br-PBI, NPBI** and **Br-NPBI** computed at the TD-CAM-B3LYP/aug-cc-pVDZ levels of theory**.**

SOC (cm^{-1})				
States	**PBI**	**Br-PBI**	**NPBI**	**Br-NPBI**
S_1/T_1	0	2.70	0	0.01
S_1/T_2	0	7.93	0.65	0.57
S_1/T_3	0.03	2.21	0.08	0.06
S_1/T_4	0.01	12.85	0.04	0.05
S_1/T_5	0.32	29.43	0.01	0.03
S_1/T_6	0	2.70	0	0.01

Section 4: Figures

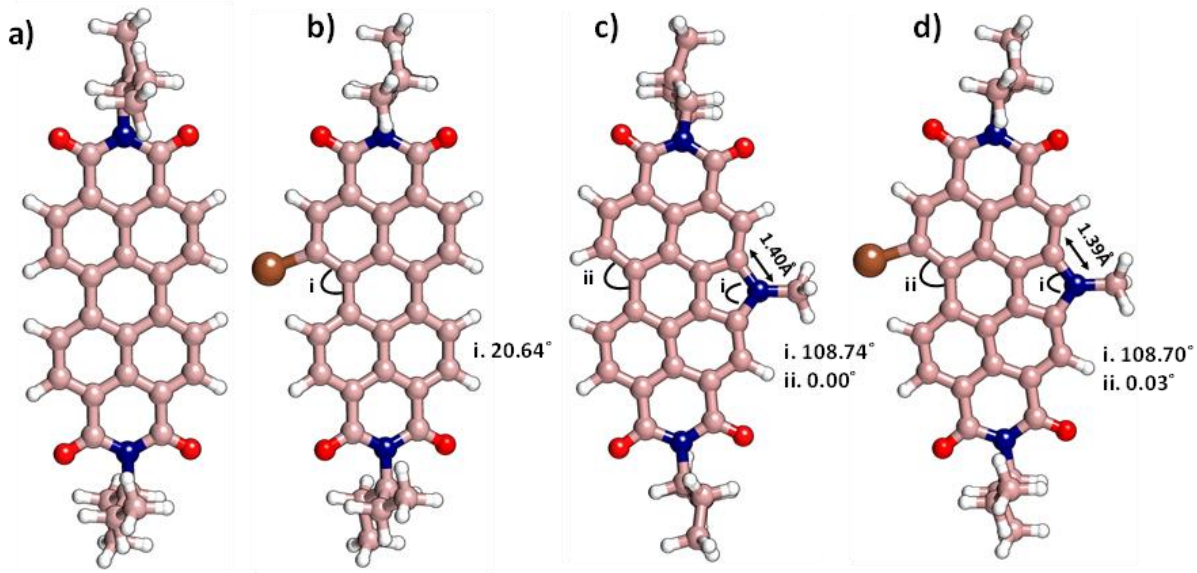


Figure S1: Optimized structures of a) **PBI** b) **Br-PBI** c) **NPBI** and d) **Br-NPBI**.[5]

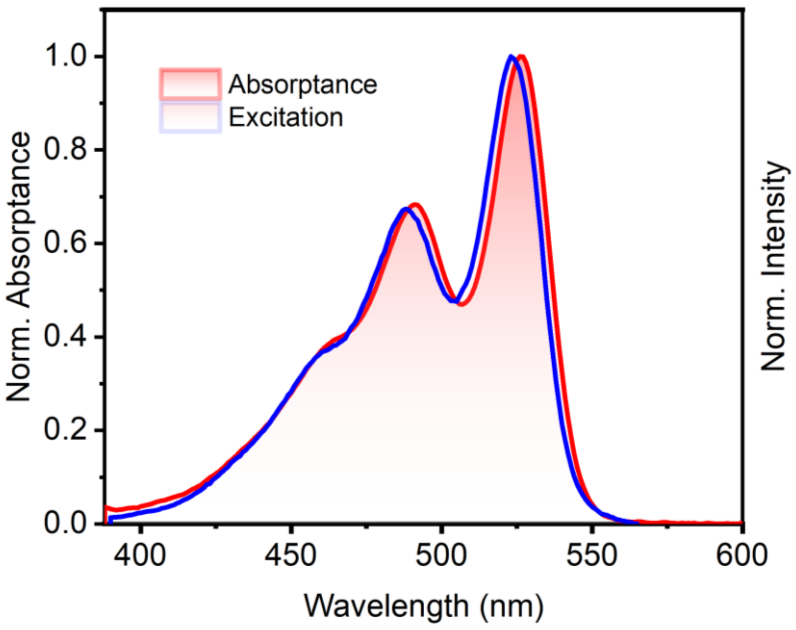


Figure S2: Normalized absorptance spectra and excitation spectra (λ_{ex}= 590 nm) of **Br-NPBI** in toluene. λ_{max}= 0.41 OD.

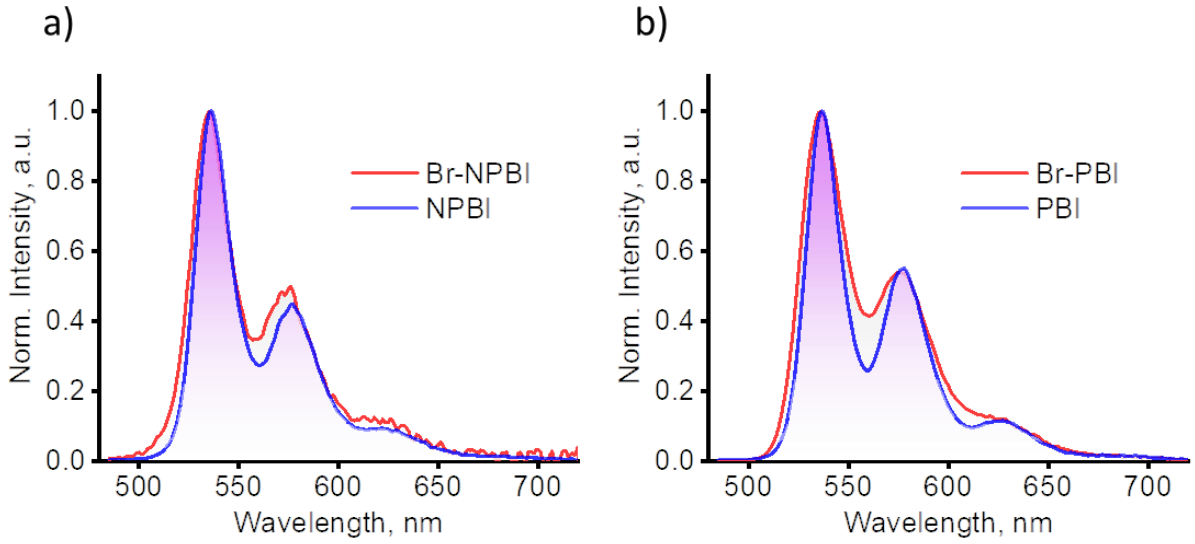


Figure S3: Normalized emission spectra of a) **NPBI** and **Br-NPBI** and b) **PBI** and **Br-PBI** in toluene.

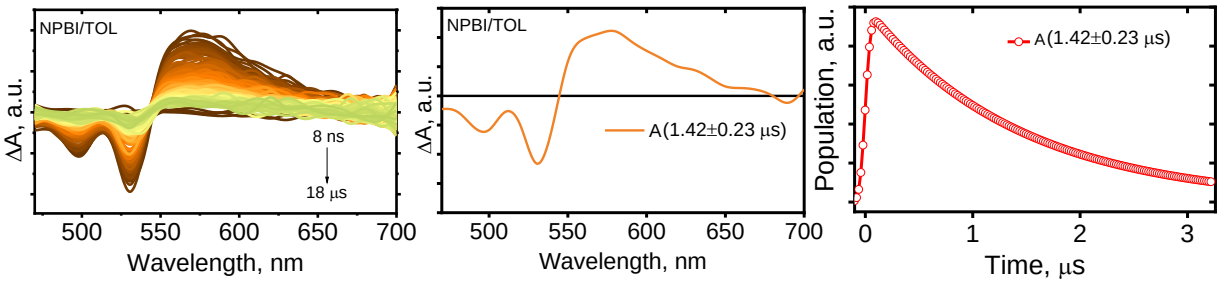


Figure S4: nsTA (λ_{ex} = 532 nm) spectrum (left), EAS (center), and the relative population profile of the triplet excited state (right) o f **NPBI** in toluene.

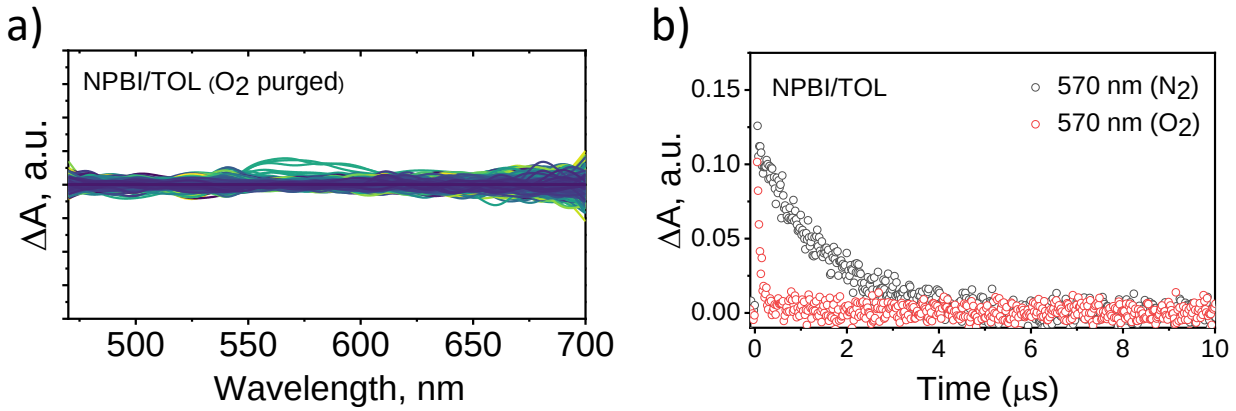


Figure S5: a) nsTA (λ_{ex} = 532 nm) spectrum of **NPBI** after oxygen purging and b) Single wavelength decay kinetics at 570 nm upon nitrogen and oxygen purging.

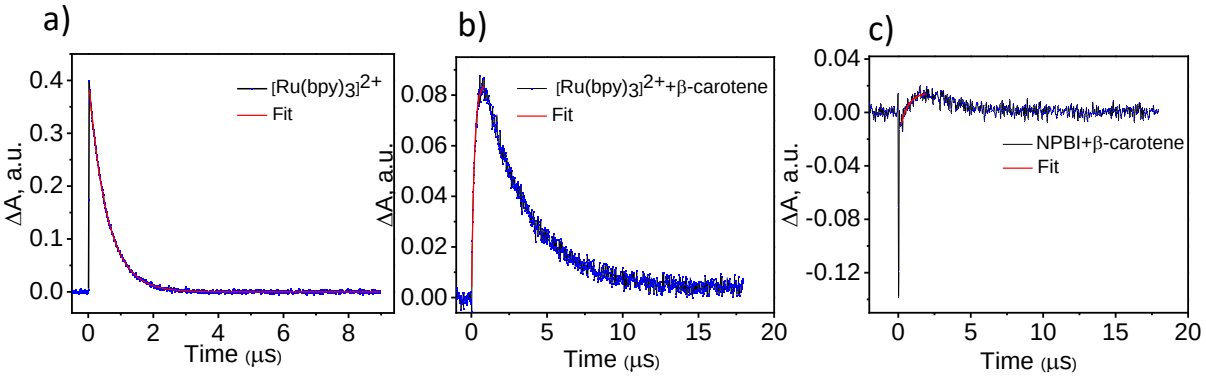


Figure S6: a) Transient kinetic decay of $[Ru(bpy)_3]^{2+}$ at 370 nm b) The growth profile of (β-carotene)* formed in the mixture of $[Ru(bpy)_3]^{2+}$ and β-carotene in toluene at 530 nm confirming the triplet–triplet energy transfer from $[Ru(bpy)_3]^{2+}$ to β-carotene c) The growth profile of (β-carotene)* formed in the mixture of **NPBI** and β-carotene in toluene at 530 nm confirming the triplet–triplet energy transfer from **NPBI** to β-carotene

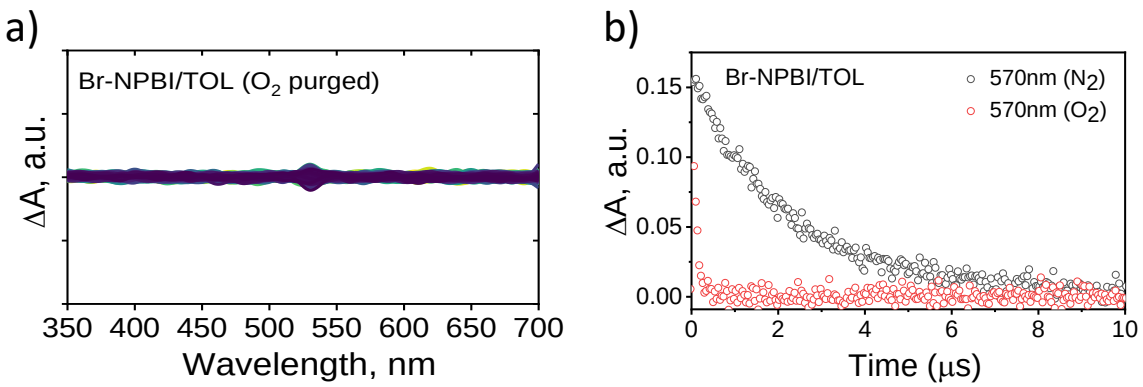


Figure S7: a) nsTA (λ_{ex} = 532 nm) spectrum of **Br-NPBI** after oxygen purging and b) Single wavelength decay kinetics at 570 nm upon nitrogen and oxygen purging.

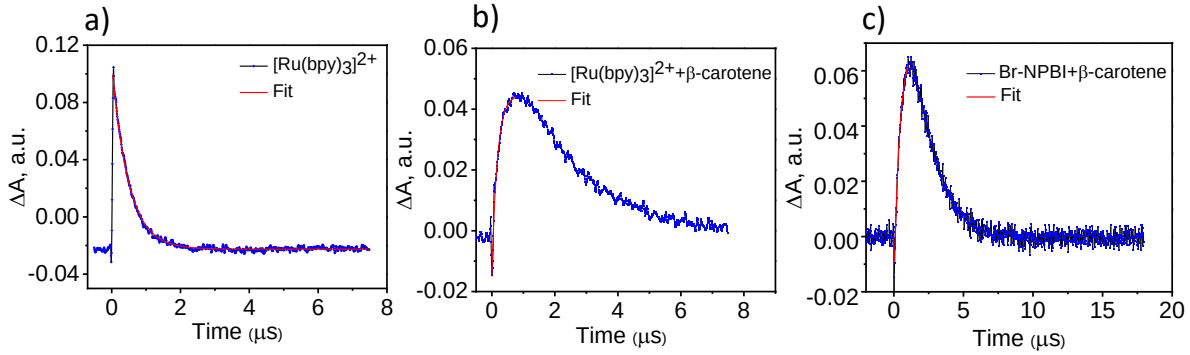


Figure S8: a) Transient kinetic decay of $[Ru(bpy)_3]^{2+}$ at 370 nm b) The growth profile of (β-carotene)* formed in the mixture of $[Ru(bpy)_3]^{2+}$ and β-carotene in toluene at 530 nm confirming the triplet–triplet energy transfer from $[Ru(bpy)_3]^{2+}$ to β-carotene c) The growth profile of (β-carotene)* formed in the mixture of **Br-NPBI** and β-carotene in toluene at 530 nm confirming the triplet–triplet energy transfer from **Br-NPBI** to β-carotene.

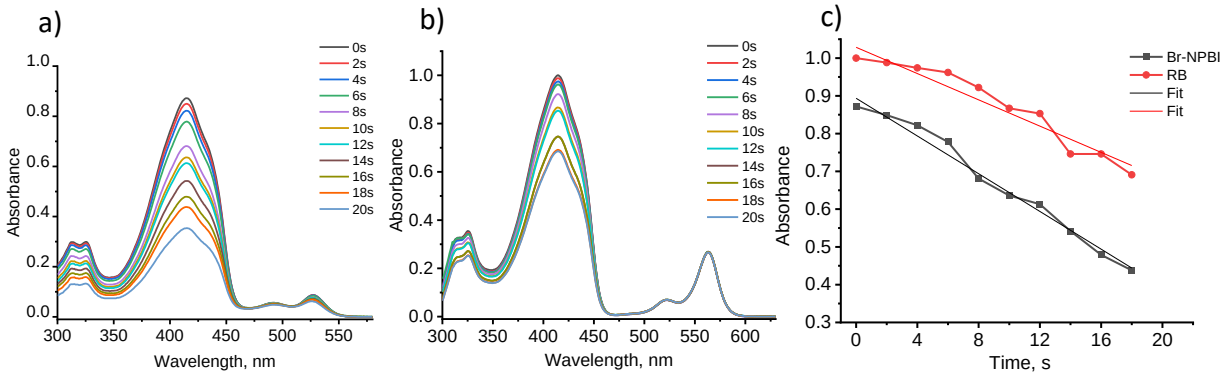


Figure S9: a) Absorption spectra of DPBF and **Br-NPBI** mixture on different irradiation time b) Absorption spectra of DPBF and Rose Bengal on different irradiation time c) Absorbance-Time plot of DPBF, DPBF with Rose Bengal, and DPBF with **Br-NPBI**.

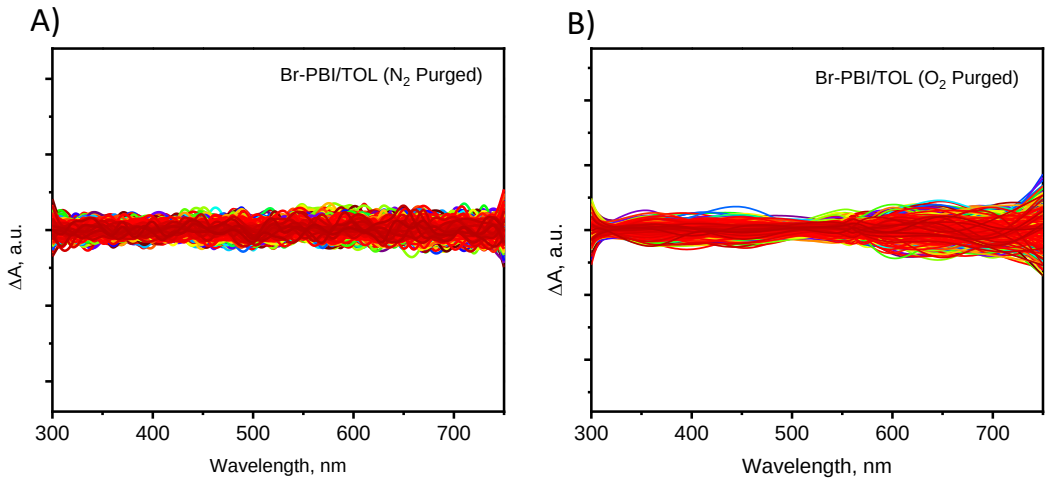


Figure S10: a) nsTA (λ_{ex} = 532 nm) spectrum of **Br-PBI** after nitrogen purging and b) oxygen purging.

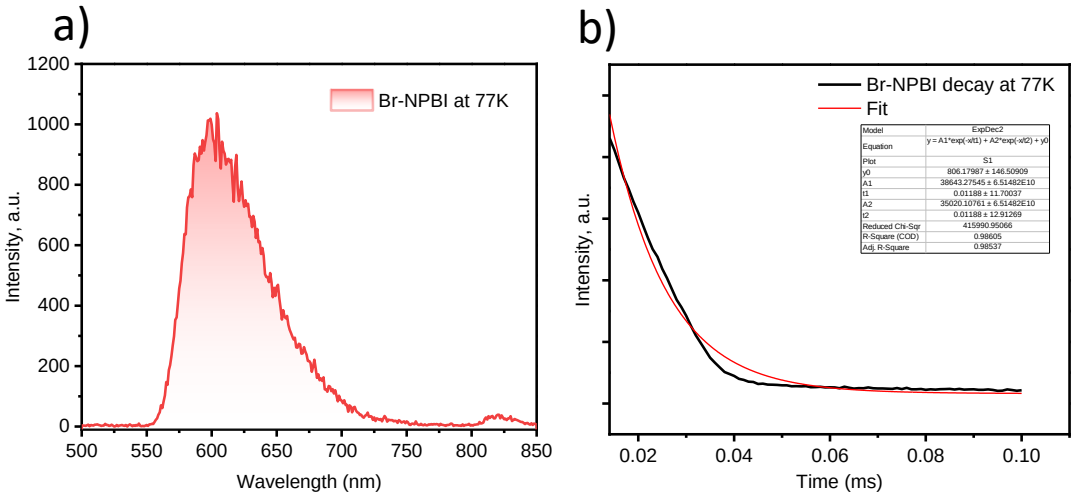


Figure S11: a) Gated emission spectrum of **Br-NPBI** at 77K and b) decay trace at 600 nm

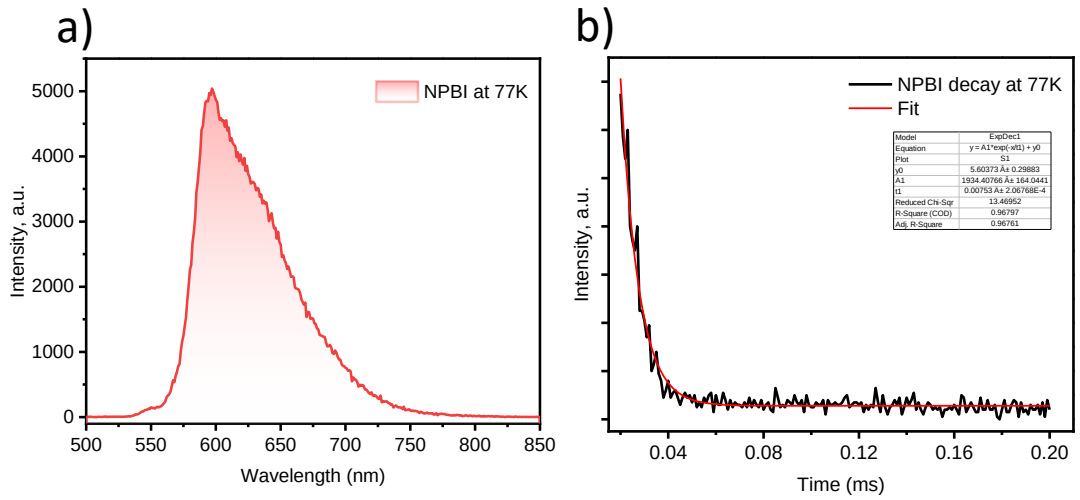


Figure S12: a) Gated emission spectrum of **NPBI** at 77K and b) decay trace at 597 nm

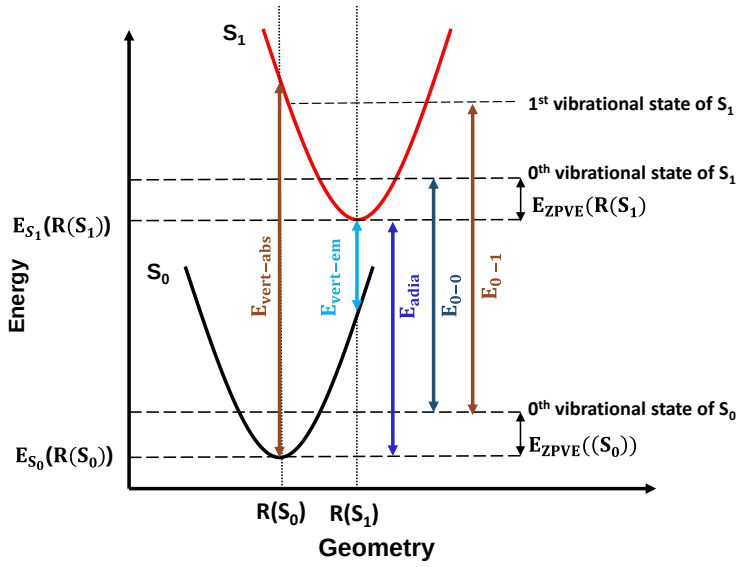


Figure S13: Energy level diagram representing the excitation energies. GS = ground state, ES = excited state, Evert = vertical excitation energy, E_{adia} = adiabatic energy, E_{ZPVE} = zero-point vibrational energy. [6,7]

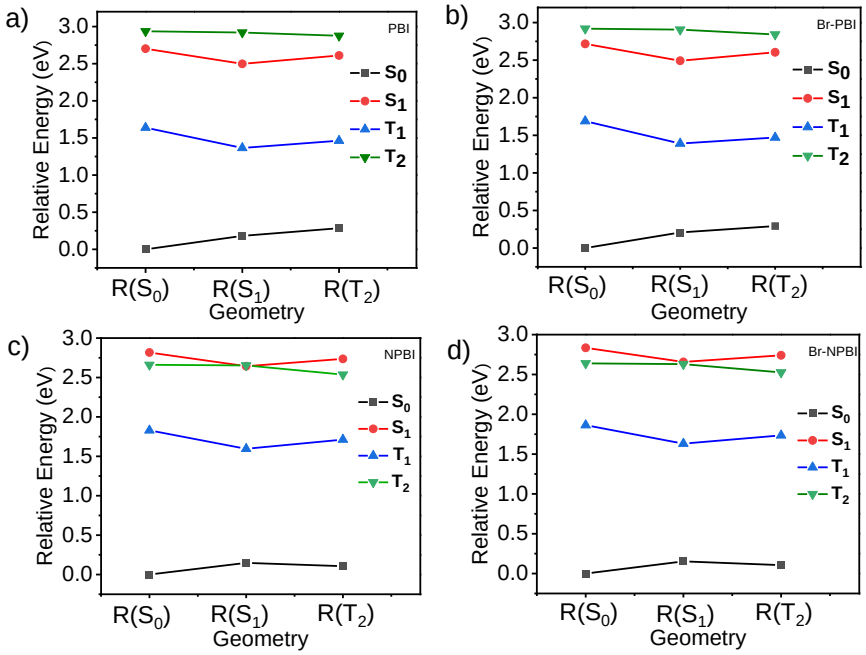


Figure S14: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0)**.** The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2: a) **PBI**, b) **Br-PBI**, c) **NPBI** and d) **Br-NPBI.** For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies. For all using at the CAM-B3LYP/aug-cc-pVDZ level of theory.

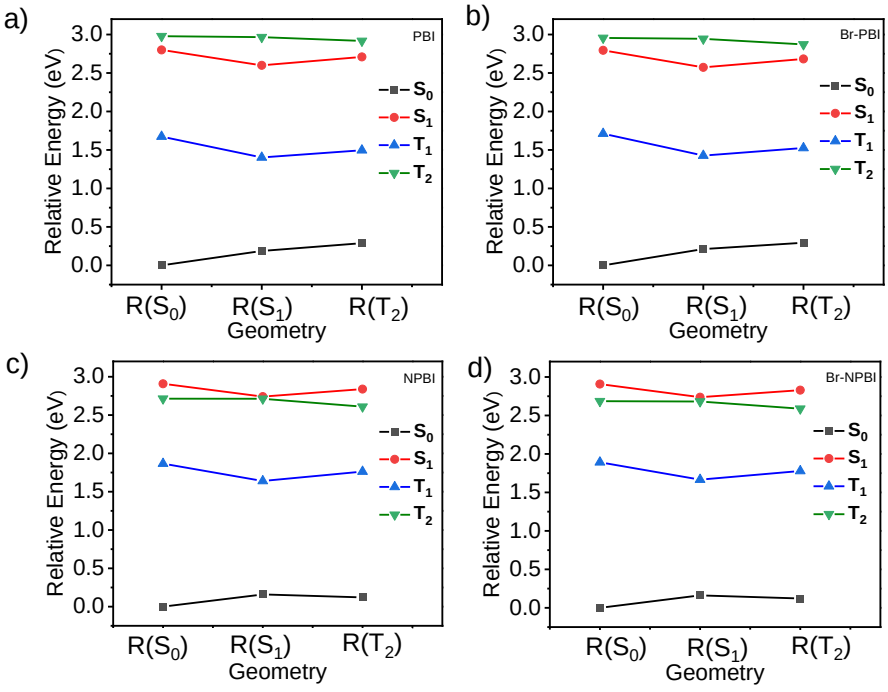


Figure S15: Energies for S_0, S_1, T_1, and T_2 states relative to the ground state energy at the ground state equilibrium geometry R(S_0). The calculations were performed for the equilibrium geometries of S_0, S_1, and T_2: a) **PBI**, b) **Br-PBI**, c) **NPBI** and d) **Br-NPBI.** For the $S_0 \rightarrow S_n$ transitions TD-DFT was employed while TDA for used for $S_0 \rightarrow T_n$ excitation energies. For all using at the CAM-B3LYP/def2-SVP level of theory.

Section 5: Cartesian Coordinates of Systems

Br-NPBI Ground State (S_0)

C	2.93415300	2.29051600	-0.05057700
C	1.53271700	2.46840500	-0.05216000
C	0.63817500	1.38408000	-0.05715700
C	1.31414800	0.11165300	-0.06137400
C	2.70427900	-0.09109700	-0.05905500
C	3.52624000	1.04056100	-0.05342100
C	0.57955400	-1.06408800	-0.06800700
C	1.03228100	-2.37773300	-0.06762900
C	2.43458200	-2.56303300	-0.06761400
C	3.23071700	-1.42150100	-0.06220000
C	-0.87001000	1.37023000	-0.05730900
C	-1.53219600	0.09863200	-0.06205300
C	-0.79513600	-1.07147900	-0.06846100
C	-1.74743500	2.46060900	-0.05200700
C	-3.14590000	2.28890900	-0.05116900
C	-3.74441000	1.03729700	-0.05459000
C	-2.92322600	-0.09633500	-0.06010200
C	-3.44552800	-1.43006500	-0.06333600
C	-2.64658600	-2.57019200	-0.06833600
C	-1.24247900	-2.38469600	-0.06825200
C	4.70935600	-1.58626600	-0.06296200
N	5.49774200	-0.42713100	-0.05175300
C	5.00185700	0.88853200	-0.05095000
C	-5.21927100	0.87696200	-0.05476600
N	-5.71365600	-0.43400100	-0.05408300
C	-4.92305400	-1.59927600	-0.06254200
O	5.73841600	1.84937400	-0.04651600
O	5.21965100	-2.68681100	-0.07091300
O	-5.96333100	1.83336800	-0.05413000
O	-5.42896800	-2.70132200	-0.06677000
C	6.97625200	-0.57685800	-0.04426100
C	-7.18629700	-0.63159500	-0.04809400
C	7.48355100	-1.26027500	1.22982000
C	7.47972100	-1.21025800	-1.34710000
C	8.98243500	-1.05315300	-1.55294100
C	6.99887500	-0.60306800	2.51656100
C	-7.83687700	-0.09464700	1.23113900
C	-7.82251300	-0.11818600	-1.34579100
C	-7.21580500	-0.63731300	2.51266600
C	-9.24934200	-0.61344400	-1.55558600
N	-0.10258600	-3.19739100	-0.06046100
C	-0.09751900	-4.64108100	-0.11590800
Br	1.00844000	4.29239400	-0.04713500
H	3.58421700	3.16561900	-0.04642900
H	2.93250400	-3.53375400	-0.07279700
H	-1.36869100	3.47721100	-0.04826200
H	-3.79552900	3.16570700	-0.04738600

H	-3.14304600	-3.54161300	-0.07292300
H	7.33138400	0.46026200	-0.02619400
H	-7.29285400	-1.72253300	-0.04036000
H	7.20831800	-2.32384000	1.21479900
H	8.58303200	-1.21664000	1.19758300
H	7.20010800	-2.27238900	-1.37446000
H	6.95148600	-0.72160700	-2.18207800
H	9.28080500	-1.43660900	-2.53967500
H	9.28880500	0.00375400	-1.50059200
H	9.56406900	-1.60675600	-0.80107900
H	7.45601900	-1.07816100	3.39692900
H	7.25129600	0.46844900	2.54279700
H	5.90741100	-0.68802200	2.63193400
H	-7.81083400	1.00377400	1.22760200
H	-8.89767400	-0.38672700	1.19559400
H	-7.79389000	0.97997500	-1.36316500
H	-7.19667200	-0.46480400	-2.18436900
H	-7.76854700	-0.28663000	3.39656400
H	-7.21870000	-1.73841700	2.52793200
H	-6.17206100	-0.30809300	2.63083600
H	-9.62807900	-0.29970600	-2.53939300
H	-9.30557400	-1.71291100	-1.51280900
H	-9.94204600	-0.21443100	-0.79993000
H	-0.98573700	-5.03442200	0.39609700
H	-0.09429300	-5.01313300	-1.15312200
H	0.79086700	-5.02906900	0.39992700

Br-NPBI First Singlet Excited State (S_1)

C	2.92411600	2.30687000	-0.04907200
C	1.54301600	2.49005500	-0.04781300
C	0.62163400	1.38080200	-0.05010800
C	1.30238400	0.11916100	-0.05227500
C	2.69986900	-0.08759200	-0.05378900
C	3.52670600	1.04311000	-0.05224100
C	0.57251900	-1.05905600	-0.05430200
C	1.03645200	-2.39440100	-0.05518400
C	2.41314600	-2.58187700	-0.06141900
C	3.21696000	-1.40941200	-0.05798100
C	-0.85263000	1.36819000	-0.05085100
C	-1.52052000	0.10561900	-0.05277800
C	-0.78733900	-1.06590900	-0.05442700
C	-1.75479300	2.47934000	-0.05081500
C	-3.13213900	2.30564600	-0.05268500
C	-3.74281700	1.03810800	-0.05451700
C	-2.91828900	-0.09200900	-0.05493300
C	-3.43312200	-1.42008200	-0.05921700
C	-2.62792900	-2.58809300	-0.06214600
C	-1.24723600	-2.40322400	-0.05555800
C	4.69135200	-1.57927000	-0.06349200
N	5.48136500	-0.42910200	-0.05810100

C	4.98886100	0.89340700	-0.05461100
C	-5.20522200	0.88064700	-0.05930400
N	-5.69761200	-0.43581500	-0.05934500
C	-4.90661300	-1.59310000	-0.06372400
O	5.73673000	1.85045100	-0.05185800
O	5.18737700	-2.69119800	-0.07078800
O	-5.95785700	1.83513000	-0.06192900
O	-5.39993100	-2.70547200	-0.06872400
C	6.95854800	-0.58433700	-0.05685400
C	-7.16947200	-0.63813900	-0.05718700
C	7.46735400	-1.26455300	1.21828200
C	7.45248100	-1.22667100	-1.35892800
C	8.95569900	-1.08276300	-1.57079200
C	6.99531100	-0.59469000	2.50325300
C	-7.82383200	-0.10070900	1.21991800
C	-7.80247900	-0.12678900	-1.35723100
C	-7.20353600	-0.64036800	2.50309200
C	-9.23036400	-0.61852600	-1.56796700
N	-0.10561200	-3.21442200	-0.04485700
C	-0.09624200	-4.65731400	-0.08987600
Br	1.00997800	4.30705300	-0.04194600
H	3.58185900	3.17633100	-0.04739000
H	2.92000600	-3.54670400	-0.06980900
H	-1.37082000	3.49404400	-0.04980500
H	-3.78735600	3.17827700	-0.05314900
H	-3.13362600	-3.55359000	-0.07035500
H	7.31674300	0.45194400	-0.04532600
H	-7.27338900	-1.72949100	-0.04859800
H	7.18190900	-2.32568400	1.21103200
H	8.56705300	-1.23149100	1.18004400
H	7.16377500	-2.28659600	-1.38133000
H	6.92530600	-0.73636400	-2.19360600
H	9.24727100	-1.47110000	-2.55771100
H	9.27092100	-0.02828600	-1.52214000
H	9.53556300	-1.63929600	-0.81969700
H	7.45259100	-1.06797500	3.38462300
H	7.25681500	0.47476100	2.52045300
H	5.90363900	-0.66881100	2.62415500
H	-7.79836900	0.99765500	1.21416600
H	-8.88408000	-0.39482500	1.18304000
H	-7.76960500	0.97117600	-1.37661200
H	-7.17614600	-0.47746400	-2.19379900
H	-7.75877100	-0.29040100	3.38577300
H	-7.20314100	-1.74152100	2.51951300
H	-6.16104800	-0.30752200	2.62236400
H	-9.60613700	-0.30743400	-2.55379200
H	-9.29024900	-1.71768600	-1.52106200
H	-9.92336800	-0.21437600	-0.81531600
H	-1.01243500	-5.04518900	0.37454000
H	-0.03499100	-5.03700800	-1.12279600

H	0.76231800	-5.04058500	0.47839000

Br-NPBI Second Triplet Excited State (T_2)

C	2.93030500	2.28661400	-0.04854400
C	1.53685200	2.47993600	-0.04801900
C	0.62971400	1.39436700	-0.05104500
C	1.30857100	0.11791100	-0.05408700
C	2.71770700	-0.10055400	-0.05507800
C	3.54011600	1.02905500	-0.05170300
C	0.58290200	-1.04346500	-0.05670300
C	1.04927100	-2.37460100	-0.05969300
C	2.42866400	-2.58127200	-0.06301600
C	3.24128200	-1.42615700	-0.05921900
C	-0.85926900	1.38349800	-0.05142700
C	-1.52809700	0.10508400	-0.05468900
C	-0.80133500	-1.05057700	-0.05708800
C	-1.74766700	2.47263600	-0.04909800
C	-3.14188400	2.28588500	-0.05030500
C	-3.75904400	1.02907300	-0.05321200
C	-2.93983500	-0.10324100	-0.05611900
C	-3.45960700	-1.42925500	-0.06023600
C	-2.64234100	-2.58292700	-0.06333200
C	-1.26305700	-2.37663600	-0.06012500
C	4.70565900	-1.59455900	-0.06324400
N	5.49351100	-0.43524500	-0.05667100
C	5.00079500	0.88463800	-0.05301000
C	-5.22093700	0.87766200	-0.05666200
N	-5.71320200	-0.43634500	-0.05839400
C	-4.92300800	-1.60212900	-0.06294200
O	5.74442400	1.84598600	-0.04930700
O	5.21487300	-2.70137100	-0.07026100
O	-5.96947500	1.83598100	-0.05680600
O	-5.42843000	-2.70966300	-0.06683000
C	6.97035800	-0.58549400	-0.05439500
C	-7.18418600	-0.63629100	-0.05672000
C	7.48164500	-1.26429900	1.22067000
C	7.46838300	-1.22592400	-1.35596600
C	8.97085100	-1.07409400	-1.56745000
C	7.00612700	-0.59668600	2.50551100
C	-7.83839100	-0.10300400	1.22229200
C	-7.81804100	-0.11928300	-1.35421300
C	-7.22140000	-0.65187800	2.50316400
C	-9.24502500	-0.61236100	-1.56788400
N	-0.10236200	-3.17697500	-0.05567600
C	-0.10174900	-4.61920000	-0.09420200
Br	1.01907700	4.30342200	-0.04289200
H	3.58751700	3.15750700	-0.04641000
H	2.92240300	-3.55339100	-0.06948800
H	-1.37781000	3.49225400	-0.04655400

H	-3.79638400	3.16005200	-0.04921700
H	-3.13459100	-3.55599800	-0.06873100
H	7.32562100	0.45181900	-0.04243500
H	-7.28882900	-1.72759300	-0.05237300
H	7.19915600	-2.32602100	1.21253400
H	8.58127900	-1.22662300	1.18334900
H	7.18426500	-2.28692500	-1.37753700
H	6.93892000	-0.73862000	-2.19098500
H	9.26528600	-1.46179500	-2.55383200
H	9.28053800	-0.01790300	-1.51951500
H	9.55341100	-1.62666900	-0.81546600
H	7.46511100	-1.06781700	3.38721500
H	7.26240000	0.47406700	2.52275900
H	5.91472900	-0.67607100	2.62519100
H	-7.80834800	0.99526400	1.22230700
H	-8.89977900	-0.39278000	1.18319200
H	-7.78674800	0.97876000	-1.36842000
H	-7.19094000	-0.46504300	-2.19225000
H	-7.77574000	-0.30445500	3.38747600
H	-7.22485100	-1.75306000	2.51308600
H	-6.17754700	-0.32410900	2.62422500
H	-9.62168800	-0.29664600	-2.55195500
H	-9.30286100	-1.71187300	-1.52677000
H	-9.93882200	-0.21377600	-0.81294800
H	-0.96901900	-5.00352300	0.45815600
H	-0.15449900	-4.98110400	-1.13397000
H	0.81738400	-5.00005400	0.36813000

Br-PBI Ground State (S0)

C	2.81600200	1.99524300	-0.11953700
C	1.40799900	2.03654600	-0.12462900
C	0.63306300	0.87733800	-0.01565800
C	1.33921800	-0.37759500	-0.08131100
C	2.75845500	-0.40430000	-0.05416300
C	3.48652400	0.80329200	-0.04515000
C	0.64992100	-1.62317500	-0.21235800
C	1.38013800	-2.80446400	-0.21356700
C	2.77580400	-2.81395600	-0.12355700
C	3.46612200	-1.62432400	-0.05912500
C	-0.83670000	0.82064400	0.15812500
C	-1.51659200	-0.41177400	-0.10760800
C	-0.81228900	-1.62319200	-0.35949600
C	-1.59699900	1.89221900	0.60710600
C	-2.99752900	1.83444100	0.68295600
C	-3.67051700	0.69764700	0.30435900
C	-2.93657000	-0.44530700	-0.08085600
C	-3.63146500	-1.62843800	-0.41157200
C	-2.92798000	-2.76813900	-0.73485600
C	-1.52856500	-2.76542600	-0.69084900
C	4.95241400	-1.65018400	-0.00236300

N	5.62053100	-0.42583500	0.02852800
C	4.97374800	0.81407400	-0.00612200
C	-5.15757700	0.67946700	0.34011100
N	-5.79534600	-0.50344900	-0.03132500
C	-5.11761300	-1.66871900	-0.41367200
O	5.59037600	1.85636000	-0.00254300
O	5.55826800	-2.69985700	0.01634600
O	-5.78715600	1.65831100	0.67925400
O	-5.71447400	-2.67455000	-0.72984000
C	7.10454400	-0.41407200	0.08717600
C	-7.27924400	-0.55518800	-0.02373800
C	7.63433400	-1.03825800	1.38200300
C	7.71420600	-0.99677600	-1.19360700
C	9.20050200	-0.69301600	-1.34703900
C	7.04294100	-0.42902700	2.64749100
C	-7.85452700	-0.38522700	1.38605800
C	-7.87237300	0.39742400	-1.06891700
C	-7.27863200	-1.35757000	2.40847300
C	-9.34655700	0.13523200	-1.35702500
Br	0.73867600	3.79549900	-0.40236000
H	3.39405800	2.91757500	-0.17144200
H	0.86293000	-3.76013500	-0.28248300
H	3.33805800	-3.74849800	-0.11922600
H	-1.11466900	2.81312700	0.91464100
H	-3.57301000	2.69548500	1.02534200
H	-3.48343800	-3.66863600	-0.99961200
H	-1.00473700	-3.69189800	-0.92162000
H	7.34524900	0.65555400	0.10970400
H	-7.49527500	-1.57946100	-0.35029900
H	7.46750600	-2.12418700	1.36434000
H	8.72432000	-0.88498200	1.38598900
H	7.54131400	-2.08147200	-1.22441200
H	7.17050000	-0.56431600	-2.04936500
H	9.56927100	-1.04537200	-2.32141400
H	9.39955300	0.38888500	-1.28779600
H	9.80679700	-1.18698600	-0.57351300
H	7.51424300	-0.85450800	3.54549400
H	7.18752600	0.66225800	2.67628800
H	5.96196300	-0.62156400	2.72672700
H	-7.71254600	0.65187000	1.72034700
H	-8.94047100	-0.54783100	1.30874600
H	-7.72613700	1.43753500	-0.74621000
H	-7.29760100	0.27085100	-2.00090200
H	-7.78070500	-1.24811800	3.38089700
H	-7.39723100	-2.40291000	2.08335400
H	-6.20469900	-1.18369400	2.57667400
H	-9.70080400	0.77569700	-2.17795900
H	-9.52001700	-0.91155400	-1.65344100
H	-9.98323800	0.34505000	-0.48490600

Br-PBI First Singlet Excited State (S_1)

C	2.79272500	2.02887800	-0.01981600
C	1.41082200	2.06345600	-0.09434000
C	0.62033600	0.86348600	-0.03503500
C	1.32963000	-0.37501900	-0.15561000
C	2.75637800	-0.39183800	-0.09976200
C	3.47162600	0.81478900	0.02218500
C	0.64549700	-1.61109400	-0.33326800
C	1.39957100	-2.81288500	-0.41331300
C	2.77405300	-2.81108800	-0.32133100
C	3.46326700	-1.60328600	-0.16547500
C	-0.80931800	0.80854600	0.14515400
C	-1.49197900	-0.41469700	-0.13003000
C	-0.79021100	-1.61269000	-0.42609700
C	-1.58063200	1.89800200	0.64182500
C	-2.95891800	1.84311800	0.71139600
C	-3.64357100	0.69282400	0.31506700
C	-2.91881800	-0.44687200	-0.08261000
C	-3.61363100	-1.62398600	-0.41443100
C	-2.90831700	-2.77972600	-0.76537500
C	-1.52911400	-2.77991800	-0.75782400
C	4.94144600	-1.62937700	-0.07401300
N	5.59978800	-0.40967500	0.07040000
C	4.94688500	0.82843400	0.11228900
C	-5.12200500	0.67656700	0.36890400
N	-5.76528400	-0.50390300	-0.00228100
C	-5.09351800	-1.66664600	-0.39673900
O	5.56024800	1.87167500	0.21826600
O	5.55199300	-2.67949500	-0.12279100
O	-5.74792900	1.65740700	0.72109600
O	-5.69288900	-2.67659600	-0.70741700
C	7.08078400	-0.39671200	0.17437500
C	-7.24887100	-0.55521100	0.02388200
C	7.57492000	-1.11955800	1.43143900
C	7.73111300	-0.87492700	-1.12947700
C	9.22077800	-0.56045400	-1.21268400
C	6.94328500	-0.61201500	2.72213400
C	-7.80492600	-0.39230800	1.44218600
C	-7.85383600	0.40420500	-1.00818300
C	-7.21610800	-1.37111100	2.45101400
C	-9.33325600	0.14932100	-1.27529100
Br	0.69090900	3.76474400	-0.50377600
H	3.37945800	2.94724700	-0.03713400
H	0.88326500	-3.76416500	-0.52833800
H	3.35351300	-3.73362600	-0.36702200
H	-1.07893100	2.78860700	1.00666500
H	-3.53988900	2.68702800	1.08498600
H	-3.47857700	-3.67125700	-1.02808200
H	-1.00351800	-3.69569100	-1.02272000

H	7.31369300	0.66888800	0.28824900
H	-7.46953000	-1.57769400	-0.30552000
H	7.41230100	-2.20097600	1.32357600
H	8.66376700	-0.96547500	1.48027700
H	7.56098400	-1.95356800	-1.25216200
H	7.21279500	-0.37488000	-1.96391600
H	9.61962200	-0.83265000	-2.20087300
H	9.41583900	0.51298000	-1.05970400
H	9.80443700	-1.11591500	-0.46382400
H	7.38931400	-1.10498800	3.59836200
H	7.08166200	0.47411600	2.83958800
H	5.86125700	-0.81236600	2.75294700
H	-7.65620300	0.64279600	1.77981500
H	-8.89211800	-0.55296200	1.37899600
H	-7.69792100	1.44210000	-0.68285300
H	-7.29352500	0.27921100	-1.94917000
H	-7.70507500	-1.26731100	3.43076100
H	-7.33939200	-2.41439700	2.12107800
H	-6.13991400	-1.19856100	2.60576000
H	-9.69679600	0.79400600	-2.08887100
H	-9.51570700	-0.89574600	-1.57246400
H	-9.95605000	0.35908200	-0.39318700

Br-PBI Second Triplet Excited State (T_2)

C	2.80283100	2.03159300	0.00417100
C	1.41846800	2.08033400	-0.10911900
C	0.60918700	0.88338300	-0.06931200
C	1.33466400	-0.36997600	-0.20478200
C	2.72994900	-0.39168100	-0.12235600
C	3.46851100	0.81960700	0.04597900
C	0.63213900	-1.60699200	-0.42775100
C	1.39822700	-2.79851900	-0.56017600
C	2.78037000	-2.79790200	-0.44931500
C	3.46007500	-1.61039800	-0.22510100
C	-0.80918200	0.83082400	0.11728400
C	-1.50557000	-0.39680300	-0.16913400
C	-0.78512200	-1.60610100	-0.50011500
C	-1.57935800	1.91288000	0.60485800
C	-2.96703600	1.85003900	0.69195000
C	-3.64270100	0.70423600	0.31412400
C	-2.90501400	-0.43289500	-0.10242200
C	-3.62387400	-1.62443600	-0.43351700
C	-2.92276600	-2.77099500	-0.80676300
C	-1.54305600	-2.77025100	-0.82978900
C	4.93600000	-1.63474300	-0.10824800
N	5.59201000	-0.42128600	0.10424200

C	4.94037100	0.81815700	0.17205200
C	-5.12484700	0.67786200	0.38690000
N	-5.76874800	-0.50379500	0.02432200
C	-5.09751000	-1.66643100	-0.38673900
O	5.55617500	1.85291000	0.32599800
O	5.55115900	-2.67862900	-0.18982600
O	-5.74893600	1.65361300	0.74920400
O	-5.70489400	-2.67385600	-0.69026500
C	7.06926300	-0.41589300	0.24632700
C	-7.25075900	-0.56100800	0.07388300
C	7.53251000	-1.19624600	1.48082800
C	7.75372400	-0.83354000	-1.06117900
C	9.24481900	-0.51637200	-1.09108200
C	6.86725200	-0.74980600	2.77715500
C	-7.78674800	-0.40190000	1.50055600
C	-7.87725800	0.39600300	-0.94787200
C	-7.17748200	-1.37774200	2.50003300
C	-9.35865100	0.13159000	-1.19384600
Br	0.73130200	3.78706100	-0.54233100
H	3.39382400	2.94750900	0.01836800
H	0.89232700	-3.74639600	-0.73242100
H	3.35770000	-3.71913900	-0.53487400
H	-1.08448600	2.81651700	0.94548100
H	-3.54538300	2.69856500	1.05946300
H	-3.49403000	-3.66317900	-1.06523200
H	-1.02743000	-3.68543000	-1.11447400
H	7.30029800	0.64270500	0.41511000
H	-7.47267400	-1.58397900	-0.25277300
H	7.37556100	-2.27169900	1.31919500
H	8.61934300	-1.04316300	1.56458200
H	7.58767500	-1.90519400	-1.23828000
H	7.25689700	-0.29494500	-1.88460600
H	9.66923100	-0.74246800	-2.08022700
H	9.43519800	0.54866000	-0.88330900
H	9.80925900	-1.10646000	-0.35408800
H	7.29225600	-1.28220200	3.64063100
H	7.00033300	0.32986600	2.94836300
H	5.78527900	-0.95256000	2.77153300
H	-7.63960100	0.63380000	1.83692700
H	-8.87374200	-0.56909300	1.45326200
H	-7.72386000	1.43456900	-0.62354200
H	-7.32990700	0.27609800	-1.89709400
H	-7.65278800	-1.27752200	3.48682200
H	-7.29939300	-2.42151900	2.17114100

H	-6.10020900	-1.19903400	2.63929000
H	-9.73843500	0.77519200	-2.00082700
H	-9.53832600	-0.91417200	-1.49021300
H	-9.96989400	0.33553400	-0.30235300

N-PBI Ground State (S_0)

C	-2.92949000	-2.85834700	-0.09036400
C	-1.52497100	-2.97135900	-0.09405700
C	-0.70970100	-1.83846600	-0.08769000
C	-1.41284600	-0.59571700	-0.07816500
C	-2.80700800	-0.45666700	-0.07266400
C	-3.57727700	-1.62626300	-0.07926300
C	-0.71032000	0.59673100	-0.07159500
C	-1.19602400	1.89463000	-0.05460000
C	-2.60931700	2.02691200	-0.05138600
C	-3.37171400	0.85994500	-0.05956800
C	0.78578300	-1.80096500	-0.08726600
C	1.42563300	-0.52439600	-0.07732700
C	0.66412900	0.63117600	-0.07120900
C	1.65675900	-2.89157000	-0.09330900
C	3.05393800	-2.70820200	-0.08900900
C	3.63868200	-1.44528200	-0.07734000
C	2.81104400	-0.31560700	-0.07103200
C	3.30947600	1.02750700	-0.05743200
C	2.48890300	2.15479900	-0.04953700
C	1.08424100	1.95179600	-0.05389300
C	-4.85478200	0.97054100	-0.05735500
N	-5.59697700	-0.21951000	-0.05976000
C	-5.05533500	-1.52115100	-0.07421900
C	5.11046200	-1.26454600	-0.07342400
N	5.58659000	0.05463300	-0.05677600
C	4.78385200	1.21375000	-0.05234000
O	-5.76396600	-2.50333200	-0.08029200
O	-5.40756100	2.05080800	-0.05164900
O	5.86927400	-2.20960700	-0.08273700
O	5.27948400	2.32046000	-0.04248500
C	-7.07964400	-0.12385700	-0.05047600
C	7.05680100	0.26980300	-0.04649400
C	-7.61225100	0.52397900	1.23198600
C	-7.60754400	0.50668600	-1.34510100
C	-9.10334300	0.29556600	-1.55315700
C	-7.10369300	-0.13160200	2.51033000

C	7.71280500	-0.27277600	1.22764900
C	7.70160400	-0.22066700	-1.34885800
C	7.08317700	0.24783600	2.51415300
C	9.12161100	0.29674000	-1.55152100
N	-0.07643800	2.74062900	-0.03644400
C	-0.11265300	4.18439600	-0.07511300
H	-3.54853300	-3.75706800	-0.09532600
H	-1.08493600	-3.97037600	-0.10153400
H	-3.14150600	2.97955400	-0.04400600
H	1.26726400	-3.91136600	-0.10117000
H	3.71775200	-3.57444600	-0.09426000
H	2.97190800	3.13321400	-0.04108600
H	-7.39674700	-1.17329400	-0.04557300
H	7.15012400	1.36176000	-0.02645000
H	-7.37623500	1.59701600	1.23110000
H	-8.70944800	0.44032400	1.19885800
H	-7.36826400	1.57885500	-1.35918800
H	-7.06151400	0.04890800	-2.18611500
H	-9.41662200	0.67988600	-2.53498000
H	-9.36959600	-0.77275800	-1.51403600
H	-9.70521300	0.81718000	-0.79433700
H	-7.57778300	0.31486500	3.39677000
H	-7.31644300	-1.21195900	2.52229600
H	-6.01604000	-0.00829700	2.62669300
H	7.70091100	-1.37131800	1.21213200
H	8.76980100	0.03338400	1.19684800
H	7.68832200	-1.31883800	-1.37826900
H	7.07191000	0.12633800	-2.18438900
H	7.63923700	-0.10525000	3.39504000
H	7.07176200	1.34865000	2.54131800
H	6.04357200	-0.09598200	2.62704400
H	9.50603200	-0.00124500	-2.53804200
H	9.16234200	1.39637600	-1.49707100
H	9.81892300	-0.10039400	-0.79909500
H	0.76539300	4.59142300	0.44388400
H	-0.12169200	4.56904200	-1.10777100
H	-1.01068800	4.54677700	0.44276400

N-PBI First Singlet Excited State (S_1)

C	-2.91074900	-2.87637200	-0.08457300
C	-1.52554900	-2.99025400	-0.08500400

C	-0.69304200	-1.83223400	-0.07512900
C	-1.40072400	-0.59994700	-0.06483100
C	-2.80145600	-0.45973200	-0.06441400
C	-3.57224100	-1.62982600	-0.07452400
C	-0.70292300	0.59413300	-0.05523400
C	-1.20242100	1.91434400	-0.04260700
C	-2.59073900	2.04759600	-0.04666600
C	-3.35941900	0.84905200	-0.05507700
C	0.76965500	-1.79512100	-0.07488300
C	1.41369700	-0.52838400	-0.06429700
C	0.65610900	0.62860900	-0.05501900
C	1.65979900	-2.90938600	-0.08474600
C	3.03759800	-2.72532500	-0.08404800
C	3.63444900	-1.44702700	-0.07329600
C	2.80552400	-0.31729800	-0.06336600
C	3.29685400	1.01768700	-0.05393000
C	2.46775800	2.17574900	-0.04564300
C	1.08810100	1.97219500	-0.04220500
C	-4.83763400	0.96140000	-0.05889600
N	-5.57953300	-0.22266400	-0.06540200
C	-5.03875400	-1.52899000	-0.07540300
C	5.09477900	-1.27025000	-0.07531600
N	5.56914300	0.05370800	-0.06226000
C	4.76644700	1.20613700	-0.05546700
O	-5.75474200	-2.51040400	-0.08249500
O	-5.38062200	2.05155700	-0.05486100
O	5.86095300	-2.21424100	-0.08644100
O	5.25124500	2.32235400	-0.04870900
C	-7.06153000	-0.12459200	-0.06297800
C	7.03862300	0.27282300	-0.05720900
C	-7.59723300	0.52180800	1.21885400
C	-7.58102400	0.51100800	-1.35847800
C	-9.07746000	0.31006100	-1.57211100
C	-7.09892500	-0.14207100	2.49700800
C	7.69898700	-0.26791900	1.21546400
C	7.67901900	-0.21863700	-1.36133500
C	7.07146700	0.25291300	2.50291800
C	9.10048000	0.29359800	-1.56679600
N	-0.07797300	2.76001300	-0.02361400
C	-0.11434800	4.20289200	-0.05504900
H	-3.53469400	-3.77165300	-0.09222900
H	-1.07778400	-3.98553200	-0.09318300
H	-3.13243500	2.99363700	-0.04515300
H	1.26300200	-3.92606900	-0.09334600

H	3.70660100	-3.58751300	-0.09221900
H	2.96004900	3.14834200	-0.04336900
H	-7.37961200	-1.17386600	-0.06221600
H	7.12990700	1.36513900	-0.03862500
H	-7.35403700	1.59338800	1.22289800
H	-8.69481100	0.44544200	1.17999500
H	-7.33436100	1.58163200	-1.37025400
H	-7.03507000	0.05032400	-2.19795900
H	-9.38451800	0.69638900	-2.55516100
H	-9.35094000	-0.75646800	-1.53388800
H	-9.67866700	0.83576200	-0.81557000
H	-7.57464700	0.30335100	3.38318400
H	-7.31753800	-1.22125300	2.50280300
H	-6.01105900	-0.02582900	2.61877100
H	7.68688700	-1.36641000	1.20012200
H	8.75561400	0.03943900	1.18194600
H	7.66050900	-1.31669600	-1.39072700
H	7.04859300	0.13143700	-2.19507800
H	7.63038600	-0.09789600	3.38297300
H	7.05753900	1.35378800	2.52882000
H	6.03298200	-0.09349300	2.61834300
H	9.48096800	-0.00374200	-2.55508200
H	9.14591600	1.39299100	-1.51006000
H	9.79830600	-0.10803500	-0.81723200
H	0.76333400	4.60582200	0.46814800
H	-0.12176500	4.59345400	-1.08577900
H	-1.01383100	4.56075200	0.46382100

Br-PBI Second Triplet Excited State (T_2)

C	-2.92788800	-2.85420200	-0.08489300
C	-1.52827900	-2.98340500	-0.08580900
C	-0.70030900	-1.84913900	-0.07675400
C	-1.40809400	-0.60277400	-0.06657200
C	-2.82184500	-0.44845600	-0.06564800
C	-3.59200300	-1.61914800	-0.07475800
C	-0.71310100	0.57596500	-0.05680900
C	-1.21515200	1.88732000	-0.04567600
C	-2.60348600	2.04253400	-0.04649000
C	-3.38351900	0.85858000	-0.05548700
C	0.77627800	-1.81234800	-0.07640300
C	1.42094700	-0.53207900	-0.06594700

C	0.66799300	0.61037100	-0.05656000
C	1.65966900	-2.90391400	-0.08514700
C	3.05119100	-2.70491400	-0.08365900
C	3.65229600	-1.43834300	-0.07296400
C	2.82521400	-0.30752100	-0.06434200
C	3.32167000	1.02597400	-0.05399200
C	2.48289100	2.16952200	-0.04518000
C	1.10414700	1.94520300	-0.04517600
C	-4.85206700	0.97415500	-0.05780300
N	-5.59495200	-0.21581800	-0.06429800
C	-5.05670500	-1.52136700	-0.07484300
C	5.11144500	-1.26609800	-0.07384300
N	5.58434700	0.05638600	-0.06141600
C	4.78115200	1.21578300	-0.05387500
O	-5.77175600	-2.50411500	-0.08192000
O	-5.40383300	2.06064300	-0.05281800
O	5.87569700	-2.21226500	-0.08349900
O	5.27652200	2.32813900	-0.04531100
C	-7.07597900	-0.11883800	-0.06133500
C	7.05259500	0.27498400	-0.05675800
C	-7.61301800	0.52595600	1.22090000
C	-7.59750400	0.51757800	-1.35573300
C	-9.09321000	0.31231800	-1.57018400
C	-7.11410700	-0.13872300	2.49838600
C	7.71355600	-0.26192700	1.21734800
C	7.69457900	-0.22017900	-1.35882700
C	7.08853300	0.26619200	2.50306000
C	9.11435100	0.29566600	-1.56689500
N	-0.07547900	2.71934200	-0.03308600
C	-0.11143700	4.16070200	-0.05826600
H	-3.55242200	-3.75005700	-0.09233000
H	-1.09748600	-3.98570000	-0.09376000
H	-3.13186700	2.99662700	-0.04178800
H	1.27931200	-3.92641900	-0.09344600
H	3.72021600	-3.56811900	-0.09132600
H	2.96218600	3.14911100	-0.03963100
H	-7.39366200	-1.16827900	-0.06151500
H	7.14320400	1.36740600	-0.04145800
H	-7.36957600	1.59731600	1.22563700
H	-8.71057500	0.44844200	1.18221400
H	-7.35317500	1.58860500	-1.36513700
H	-7.04992500	0.05995700	-2.19585500
H	-9.40180700	0.70001800	-2.55228200
H	-9.36336500	-0.75518100	-1.53441900

H	-9.69624400	0.83406700	-0.81230300
H	-7.59043000	0.30489400	3.38521900
H	-7.33090400	-1.21830300	2.50267000
H	-6.02637900	-0.02101800	2.61957400
H	7.69815500	-1.36041900	1.20672600
H	8.77098700	0.04255600	1.18183900
H	7.67913100	-1.31832900	-1.38385000
H	7.06288100	0.12471100	-2.19376800
H	7.64698700	-0.08213600	3.38447100
H	7.07694000	1.36717300	2.52343300
H	6.04909500	-0.07672400	2.61993500
H	9.49625100	-0.00507600	-2.55367100
H	9.15612800	1.39546900	-1.51519700
H	9.81349400	-0.09987200	-0.81526100
H	0.77366200	4.56112700	0.45222000
H	-0.12024300	4.53058900	-1.09679600
H	-1.01586500	4.51641700	0.45144300

PBI Ground State (S0)

C	-1.96581100	3.20065500	-0.06982600
C	-2.18082700	1.81613200	-0.07018900
C	-1.12843100	0.91152200	-0.07007900
C	0.20850600	1.41457900	-0.06981100
C	0.41575000	2.82033000	-0.06935500
C	-0.68446300	3.70533700	-0.06903900
C	1.34350800	0.54712800	-0.06991500
C	2.61218900	1.10944500	-0.06968300
C	2.80587800	2.49720400	-0.06928800
C	1.72466500	3.34977300	-0.06866100
C	-1.34350800	-0.54712800	-0.06991500
C	-0.20850600	-1.41457900	-0.06981100
C	1.12843100	-0.91152200	-0.07007900
C	-2.61218900	-1.10944500	-0.06968300
C	-2.80587800	-2.49720400	-0.06928800
C	-1.72466500	-3.34977300	-0.06866100
C	-0.41575000	-2.82033000	-0.06935500
C	0.68446300	-3.70533700	-0.06903900
C	1.96581100	-3.20065500	-0.06982600
C	2.18082700	-1.81613200	-0.07018900
C	1.95692300	4.81858700	-0.06930300
N	0.83604600	5.64817500	-0.06411000

C	-0.48392100	5.17781500	-0.06814000
C	-1.95692300	-4.81858700	-0.06930300
N	-0.83604600	-5.64817500	-0.06411000
C	0.48392100	-5.17781500	-0.06814000
O	-1.42783400	5.93761900	-0.06875300
O	3.08051500	5.27474300	-0.07247200
O	-3.08051500	-5.27474300	-0.07247200
O	1.42783400	-5.93761900	-0.06875300
C	1.02926100	7.12024000	-0.05793400
C	-1.02926100	-7.12024000	-0.05793400
C	1.72466500	7.60478200	1.21833000
C	1.68651800	7.59879700	-1.35823300
C	1.58851400	9.10626300	-1.56535800
C	1.04382400	7.14761700	2.50281900
C	-1.72466500	-7.60478200	1.21833000
C	-1.68651800	-7.59879700	-1.35823300
C	-1.04382400	-7.14761700	2.50281900
C	-1.58851400	-9.10626300	-1.56535800
H	-2.80248900	3.90044600	-0.06982800
H	-3.20958900	1.45962600	-0.07048100
H	3.49423600	0.47111000	-0.06983800
H	3.80870800	2.92636800	-0.06947800
H	-3.49423600	-0.47111000	-0.06983800
H	-3.80870800	-2.92636800	-0.06947800
H	2.80248900	-3.90044600	-0.06982800
H	3.20958900	-1.45962600	-0.07048100
H	0.00318600	7.50685000	-0.04525800
H	-0.00318600	-7.50685000	-0.04525800
H	2.77713200	7.28906600	1.20843000
H	1.72314900	8.70500600	1.18382800
H	2.73722800	7.27809300	-1.38059700
H	1.18155700	7.08916800	-2.19505900
H	1.98592100	9.38867800	-2.55124000
H	0.54411300	9.45340700	-1.51607100
H	2.16231200	9.66651600	-0.81245000
H	1.53256600	7.58731200	3.38457100
H	-0.01730100	7.44110100	2.52402600
H	1.08637900	6.05387300	2.62001700
H	-2.77713200	-7.28906600	1.20843000
H	-1.72314900	-8.70500600	1.18382800
H	-2.73722800	-7.27809300	-1.38059700
H	-1.18155700	-7.08916800	-2.19505900
H	-1.53256600	-7.58731200	3.38457100
H	0.01730100	-7.44110100	2.52402600

H	-1.08637900	-6.05387300	2.62001700
H	-1.98592100	-9.38867800	-2.55124000
H	-0.54411300	-9.45340700	-1.51607100
H	-2.16231200	-9.66651600	-0.81245000

PBI First Singlet Excited State (S_1)

C	-1.98733200	3.18162200	-0.06988000
C	-2.20403400	1.81942200	-0.07036000
C	-1.12446100	0.89359700	-0.07036700
C	0.20635100	1.39802700	-0.07012800
C	0.41484800	2.81043500	-0.06958200
C	-0.68361200	3.69039600	-0.06918200
C	1.33475800	0.53067700	-0.07023900
C	2.63590400	1.10496300	-0.07000800
C	2.82205300	2.47169400	-0.06940800
C	1.72090800	3.33505400	-0.06867400
C	-1.33475800	-0.53067700	-0.07023900
C	-0.20635100	-1.39802700	-0.07012800
C	1.12446100	-0.89359700	-0.07036700
C	-2.63590400	-1.10496300	-0.07000800
C	-2.82205300	-2.47169400	-0.06940800
C	-1.72090800	-3.33505400	-0.06867400
C	-0.41484800	-2.81043500	-0.06958200
C	0.68361200	-3.69039600	-0.06918200
C	1.98733200	-3.18162200	-0.06988000
C	2.20403400	-1.81942200	-0.07036000
C	1.95424300	4.79608300	-0.06901800
N	0.83387900	5.62558700	-0.06516500
C	-0.48571000	5.15578200	-0.06830900
C	-1.95424300	-4.79608300	-0.06901800
N	-0.83387900	-5.62558700	-0.06516500
C	0.48571000	-5.15578200	-0.06830900
O	-1.43353500	5.91629300	-0.06815300
O	3.08216400	5.25110500	-0.07100800
O	-3.08216400	-5.25110500	-0.07100800
O	1.43353500	-5.91629300	-0.06815300
C	1.02725900	7.09744000	-0.05887100
C	-1.02725900	-7.09744000	-0.05887100
C	1.72090800	7.58062100	1.21885800
C	1.68769600	7.57461200	-1.35803800
C	1.59694000	9.08275600	-1.56361600
C	1.03595200	7.12433600	2.50149800

C	-1.72090800	-7.58062100	1.21885800
C	-1.68769600	-7.57461200	-1.35803800
C	-1.03595200	-7.12433600	2.50149800
C	-1.59694000	-9.08275600	-1.56361600
H	-2.81574100	3.89072900	-0.06975300
H	-3.22967000	1.45506400	-0.07068600
H	3.51241200	0.45964100	-0.07033300
H	3.81980800	2.91178800	-0.06945900
H	-3.51241200	-0.45964100	-0.07033300
H	-3.81980800	-2.91178800	-0.06945900
H	2.81574100	-3.89072900	-0.06975300
H	3.22967000	-1.45506400	-0.07068600
H	0.00112100	7.48422100	-0.04815200
H	-0.00112100	-7.48422100	-0.04815200
H	2.77251600	7.26185100	1.21087800
H	1.72204700	8.68090500	1.18472100
H	2.73680300	7.24854700	-1.37951800
H	1.18086300	7.06821000	-2.19571300
H	1.99540000	9.36424300	-2.54938100
H	0.55423100	9.43493200	-1.51364500
H	2.17370700	9.63947600	-0.81034300
H	1.52308100	7.56289800	3.38477300
H	-0.02480300	7.41934900	2.51981900
H	1.07646900	6.03043300	2.61816300
H	-2.77251600	-7.26185100	1.21087800
H	-1.72204700	-8.68090500	1.18472100
H	-2.73680300	-7.24854700	-1.37951800
H	-1.18086300	-7.06821000	-2.19571300
H	-1.52308100	-7.56289800	3.38477300
H	0.02480300	-7.41934900	2.51981900
H	-1.07646900	-6.03043300	2.61816300
H	-1.99540000	-9.36424300	-2.54938100
H	-0.55423100	-9.43493200	-1.51364500
H	-2.17370700	-9.63947600	-0.81034300

PBI Second Triplet Excited State (T_2)

C	2.80349100	2.50394600	-0.06649200
C	1.41976900	2.49150000	-0.06632200
C	0.67906400	1.27465900	-0.06612600
C	1.42214800	0.03524300	-0.06604900
C	2.81914000	0.06960200	-0.06626300

C	3.52056400	1.31217600	-0.06623100
C	0.74077900	-1.23969700	-0.06592400
C	1.54067500	-2.41912700	-0.06611500
C	2.92291900	-2.36357300	-0.06644400
C	3.58044000	-1.13768100	-0.06607600
C	-0.74079900	1.23971500	-0.06621500
C	-1.42218000	-0.03524900	-0.06611300
C	-0.67908700	-1.27467600	-0.06587900
C	-1.54068500	2.41913400	-0.06668700
C	-2.92290600	2.36358300	-0.06707900
C	-3.58045500	1.13768300	-0.06652600
C	-2.81918000	-0.06960800	-0.06649900
C	-3.52058900	-1.31217400	-0.06620600
C	-2.80349500	-2.50395400	-0.06608500
C	-1.41979100	-2.49150700	-0.06577500
C	5.05849800	-1.11106000	-0.06846400
N	5.68549700	0.13637600	-0.06466100
C	4.99745100	1.35898600	-0.06700100
C	-5.05850100	1.11107700	-0.06876700
N	-5.68550400	-0.13636200	-0.06489000
C	-4.99746700	-1.35898000	-0.06711800
O	5.58941700	2.41905500	-0.06785000
O	5.70293500	-2.14135300	-0.07228800
O	-5.70293400	2.14137100	-0.07256800
O	-5.58944500	-2.41904400	-0.06787000
C	7.16796600	0.19610700	-0.06205700
C	-7.16797400	-0.19604200	-0.06216600
C	7.76766700	-0.40644700	1.21283400
C	7.74874400	-0.37053100	-1.36370900
C	9.21780000	-0.01973700	-1.57292900
C	7.20443500	0.18697100	2.49852700
C	-7.76748300	0.40626600	1.21292800
C	-7.74887200	0.37089300	-1.36363600
C	-7.20417500	-0.18763800	2.49837400
C	-9.21794000	0.02013800	-1.57282000
H	3.36067900	3.44144500	-0.06672100
H	0.89337400	3.44392500	-0.06644300
H	1.06142300	-3.39614200	-0.06622300
H	3.52618200	-3.27215700	-0.06714400
H	-1.06143900	3.39615400	-0.06692400
H	-3.52618100	3.27215900	-0.06791800
H	-3.36070200	-3.44144200	-0.06611600
H	-0.89340100	-3.44393500	-0.06553100
H	7.37488700	1.27290400	-0.05022200

H	-7.37495400	-1.27282900	-0.05049200
H	7.63557800	-1.49726800	1.20354000
H	8.85147700	-0.21744800	1.17544900
H	7.60944500	-1.46020700	-1.38640200
H	7.15990200	0.04198800	-2.19922600
H	9.56130800	-0.36209100	-2.56010200
H	9.38424100	1.06812200	-1.52190700
H	9.86807900	-0.49238700	-0.82210800
H	7.72356800	-0.21886000	3.37917900
H	7.31211700	1.28267300	2.51867400
H	6.13438600	-0.04189700	2.61858200
H	-7.63524500	1.49707100	1.20392500
H	-8.85132500	0.21743500	1.17561400
H	-7.60959500	1.46057600	-1.38607200
H	-7.16009000	-0.04140600	-2.19930200
H	-7.72312000	0.21799200	3.37922800
H	-7.31203100	-1.28333200	2.51818700
H	-6.13407200	0.04101200	2.61836200
H	-9.56154100	0.36277500	-2.55986300
H	-9.38437100	-1.06773400	-1.52209100
H	-9.86815300	0.49257300	-0.82180300

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