Supporting Information for

Excited-state Dynamics of Crossing Controlled Energy Transfer in Europium Complexes

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1. Computational mechanism design for the candidate antennas

Table S1. Vertical excitation energies ($\Delta E_{\perp}$, kcal mol$^{-1}$/nm), oscillator strengths ($f$), dipole moments (D.M., Debye), and the schematic representation of singly occupied orbitals for the $S_0 \rightarrow S_1(1\pi\pi^*)$ bright states of the candidate antennas of PPPD, para-Br-PPPD and meta-Br-PPPD obtained by CASPT2//CASSCF calculations.

| Transition      | D.M. | $f$  | $\Delta E_{\perp}$ | singly occupied orbitals |
|-----------------|------|------|-------------------|--------------------------|
| PPPD            |      |      |                   |                          |
| $S_0$           | 5.7  | --   | 0.0               |                          |
| $S_0 \rightarrow S_1(1\pi\pi^*)$ | 4.9  | 0.47 | 73.2/391          | $\pi$–dione              |
| para-Br-PPPD    |      |      |                   |                          |
| $S_0$           | 8.4  | --   | 0.0               |                          |
| $S_0 \rightarrow S_1(1\pi\pi^*)$ | 3.6  | 0.42 | 70.6/405          | $\pi$–dione              |
| meta-Br-PPPD    |      |      |                   |                          |
| $S_0$           | 9.0  | --   | 0.0               |                          |
| $S_0 \rightarrow S_1(1\pi\pi^*)$ | 3.1  | 0.43 | 70.7/404          | $\pi$–dione              |

Table S2. Adiabatic energies of the lowest-lying triplet $3\pi\pi^*$ state ($T_{0-0}$, kcal mol$^{-1}$) and spin–orbit couplings (SOCs cm$^{-1}$) between the triplet $3\pi\pi^*$ minima and corresponding $S_0$ states are summarized for the parent PPPD and its 9 derivatives, in which Br atoms are placed in different substituted positions of pyridine and phenyl moieties as shown in the left column of numbering scheme. Mulliken charge changes between the bright $S_{\text{CT}}(1\pi\pi^*)$ and corresponding $S_0$ states are provided on the three fragments of the pyridine ($\Delta q_I$), diketone ($\Delta q_{II}$), and phenyl moieties ($\Delta q_{III}$) upon the visible-light driven $S_0 \rightarrow S_{\text{CT}}(1\pi\pi^*)$ transitions on the basis of the CASPT2//CASSCF computations.

| PPPD | Br–position | $T_{0-0}$ | SOC | $\Delta q_I$ | $\Delta q_{II}$ | $\Delta q_{III}$ |
|------|-------------|-----------|-----|--------------|-----------------|------------------|
| PPPD | 2           | 51.0      | 12.3| 0.4281       | -0.6216         | 0.1935           |
| PPPD | 3           | 51.6      | 52.3| 0.4476       | -0.6413         | 0.1937           |
| PPPD | 4           | 53.0      | 0.8 | 0.4244       | -0.6386         | 0.2142           |
| PPPD | 5           | 53.1      | 3.1 | 0.4043       | -0.6232         | 0.2189           |
| PPPD | 6           | 45.6      | 6.4 | 0.4386       | -0.6293         | 0.1907           |
| PPPD | 2'          | 45.9      | 19.0| 0.0557       | -0.6322         | 0.5765           |
| PPPD | 3'          | 59.9      | <10$^{-3}$| 0.0209   | -0.6604         | 0.6395           |
| PPPD | 4'          | 50.4      | 0.7 | 0.0213       | -0.6577         | 0.6364           |
| PPPD | 5'          | 49.4      | 5.4 | -0.0094      | -0.6357         | 0.6453           |

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Figure S1. Minimum-energy profiles (MEPs) for the relaxation processes of the photo-excited free antenna ligands of PPPD (a), para-Br-PPPD (b) and meta-Br-PPPD (c) obtained at the CASPT2//IRC//CASSCF level of theory. Showing values along decay paths are the related barriers for the rotational deformation of pyridine or benzene ring in kcal/mol and the SOC at the singlet-triplet crossings (STCs) in cm⁻¹. Selected stationary structures are given with their rotational dihedral angles (°) in green. The singly occupied molecular orbitals are schematically shown in the left panel, which can be used to describe the visible light initiated CT excitation. This mainly accounts for the non-radiative decay of visible light irradiated free antenna ligands associated with rotational deformation of pyridine or benzene, leading to the conical intersection (CI) of S_{CT} and S_0 states, i.e., CI(S_{CT}/S_0).
2. Synthesis and characterization of ligand and Eu-complexes

2.1 Synthesis

**[Eu(PPPD)]$_2$ (1):** The water solution (2 mL) of Eu(Ac)$_3$·6H$_2$O (0.05 mmol, 21.9 mg) was added to the bottom of a test tube, and then 3 mL mixed solvent (CH$_3$OH:H$_2$O=1:1) was used as a buffer layer. Finally, 3 mL methanol solution of PPPD (0.15 mmol, 33.9 mg) was carefully transferred on the top of the solution. The resulting solution was left at room temperature for one week before giving rise to plate yellow crystals of complex 1. Yield: 18.9 mg (45.9 %) based on europium ions. Elemental analysis (%) calcd for C$_{42}$H$_{30}$EuN$_3$O$_6$ (1): C, 61.17, N, 5.09, H, 3.67; found C, 60.95, N, 5.06, H, 3.72. Selected IR (KBr, cm$^{-1}$) for 1: 3421(br), 3061(w), 1601(s), 1551(s), 1518(s), 1452(s), 1424(s), 1393(s), 1285(m), 1231(m), 1024(s), 795(w), 748(s), 691(s), 613(w).

**[Eu(para-Br-PPPD)]$_3$ (2):** Eu(Ac)$_3$·6H$_2$O (0.05 mmol, 21.9 mg) was added to a 10 mL methanol solution containing para-Br-PPPD (0.15 mmol, 45.9 mg). The resulting solution was stirred for 5 min to give a clear yellow solution. Upon filtration, the resulting yellow solution was left to evaporate at room temperature for several days before giving rise to bright yellow plate crystals of complex 2. Yield: 34.7 mg (65.4 %) based on europium ions. Elemental analysis (%) calcd for C$_{42}$H$_{27}$Br$_3$EuN$_3$O$_6$ (2): C, 47.50, N, 3.96, H, 2.54; found C, 47.52, N, 3.91, H, 2.63. Selected IR (KBr, cm$^{-1}$) for 2: 3421(br), 3064(w), 1605(s), 1560(s), 1516(s), 1451(s), 1425(s), 1396(s), 1287(m), 1231(m), 1027(s), 794(w), 747(s), 695(s), 616(w).

**[Eu$_2$(meta-Br-PPPD)$_6$(H$_2$O)(CH$_3$OH)]·H$_2$O (3):** The water solution (2 mL) of Eu(Ac)$_3$·6H$_2$O (0.05 mmol, 21.9 mg) was added to the bottom of a test tube, and then 2 mL mixed solvent (CH$_3$OH:H$_2$O=1:1) and methanol solution (3 mL) were used as a buffer layer. Finally, 3 mL methanol solution of meta-Br-PPPD (0.15 mmol, 45.9 mg) was carefully transferred on the top of the solution, giving rise to the block yellow crystals of complex 3 in a month. Yield: 19.3 mg (35.6 %) based on europium ions. Elemental analysis (%) calcd for C$_{85}$H$_{62}$Br$_6$Eu$_2$N$_6$O$_{15}$ (3): C, 46.56, N, 3.83, H, 2.83; found C, 46.55, N, 3.85, H, 2.80. Selected IR (KBr, cm$^{-1}$) for 3: 3421(br), 3060(w), 1608(s), 1560(s), 1516(s), 1456(s), 1420(s), 1392(s), 1281(m), 1232(m), 1024(s), 795(w), 746(s), 695(s), 614(w).

**[Eu$_2$(meta-Br-PPPD)$_2$(PNO)$_2$] (4):** Eu(Ac)$_3$·6H$_2$O (0.03 mmol, 13.1 mg) was added to a 10 mL methanol solution of meta-Br-PPPD (0.09 mmol, 27.5 mg) and the reaction mixture was stirred and heated at 40 °C for 5 min. Finally, solid PNO (0.09 mmol, 8.6 mg) was added to give a clear yellow solution. Upon filtration, the resulting solution was left to evaporate at room temperature for several days before giving rise to tabular yellow crystals of complex 4. Yield: 11.3 mg (30.1 %) based on europium ions. Elemental analysis (%) calcd for C$_{104}$H$_{74}$Br$_6$Eu$_2$N$_{10}$O$_{16}$ (4): C, 49.89, N, 5.60, H, 2.96; found C, 49.90, N, 5.63, H, 2.94. Selected IR (KBr, cm$^{-1}$) for 4: 3421(br), 3059 (w), 1607(s), 1558(s), 1516(s), 1463(s), 1420(s), 1395(s), 1247(s), 1232(m), 1024(s), 795(w), 770(s), 695(s), 615(w).
2.2 X-ray crystallography and physical measurements

Figure S2. Crystal structures of Eu-PPPD (1), Eu-para-Br-PPPD (2) and Eu-meta-Br-PPPD (3 and 4) complexes. Colour code: Eu (green), O (red), N (blue), C (dark grey). Hydrogen atoms are omitted for clarity.

Figure S3. The C-H···π connection between the layers in 1. Colour code: Eu (green), O (red), N (blue), C (dark grey). Hydrogen atoms are omitted for clarity.
**Figure S4.** The \( \pi \cdots \pi \) connection between the layers in 2. Colour code: Eu (green), O (red), N (blue), C (dark grey), Br (orange). Hydrogen atoms are omitted for clarity.

**Figure S5A.** The coordination polyhedron around Eu\(^{13+}\) ion (a) and Eu\(^{23+}\) ion (b) of complex 3. Colour code: Eu (green), O (red), N (blue).
**Figure S5B.** 1D chain of complex 3 constructed by hydrogen bonds. Colour code: Eu (green), O (red), N (blue). Most hydrogen atoms, bromine atoms and the guest water molecules are omitted for clarity.

**Figure S5C.** The π-π stackings between the chains in complex 3. Colour code: Eu (green), O (red), N (blue), C (dark grey). Most hydrogen atoms, bromine atoms and the guest water molecules are omitted for clarity.
Figure S5D. The π-π stackings between the layers in complex 3. Colour code: Eu (green), O (red), N (blue), C (dark grey). Most hydrogen atoms, bromine atoms and the guest water molecules are omitted for clarity.

Table S3. Crystallographic data and structure refinement for complex 1–3

| Complex | 1 | 2 | 3 |
|---------|---|---|---|
| Formula | C₄₂H₅₀EuN₃O₆ | C₄₂H₂₁₇Br₅EuN₃O₆ | C₆₅H₆₀Br₆Eu₂N₆O₁₅ |
| Mr | 824.65 | 1061.36 | 2190.79 |
| Crystal system | orthorhombic | orthorhombic | triclinic |
| Space group | Pbcn | Pca₂₁ | P ₁ |
| a (Å) | 16.794(7) | 29.290(9) | 11.503(3) |
| b (Å) | 25.861(8) | 16.933(5) | 19.024(5) |
| c (Å) | 8.156(5) | 7.806(3) | 21.128(4) |
| V (Å³) | 3542.7(3) | 3871.8(2) | 4145.4(1) |
| α (°) | 90 | 90 | 115.877(3) |
| β (°) | 90 | 90 | 93.390(2) |
| γ (°) | 90 | 90 | 91.574(2) |
| Z | 4 | 4 | 2 |
| Dcalc | 1.546 | 1.821 | 1.755 |
| μ (mm⁻¹) | 1.824 | 15.655 | 14.671 |
| F (000) | 1656 | 2064 | 2140 |
| GOF | 1.091 | 1.049 | 1.057 |
| Data collected | 12333 | 10072 | 28956 |
| unique | 4299 | 5819 | 15645 |
| Rint | 0.0549 | 0.0445 | 0.0388 |
| R₁, wR₂[I>2σ(I)] | 0.0516, 0.0866 | 0.0864, 0.2225 | 0.0713, 0.1893 |
| R₁, wR₂[all data] | 0.0911, 0.0996 | 0.0997, 0.2352 | 0.0764, 0.1951 |
Table S4. Selected bond distances (Å) in complex 1−3

|     | Eu1-O3 | 2.323(3) | Eu1-O3#1 | 2.323(3) | Eu1-N1#2 | 2.635(4) |
|-----|--------|----------|----------|----------|----------|----------|
|     | Eu1-O2 | 2.363(3) | Eu1-O2#1 | 2.363(3) | Eu1-N1#3 | 2.635(4) |
|     | Eu1-O1 | 2.390(3) | Eu1-O1#1 | 2.390(3) |          |          |

|     | Eu1-O5 | 2.314(1) | Eu1-O3   | 2.370(1) | Eu1-N1#1 | 2.616(1) |
|-----|--------|----------|----------|----------|----------|----------|
|     | Eu1-O1 | 2.357(1) | Eu1-O6   | 2.386(1) | Eu1-N2#2 | 2.625(1) |
|     | Eu1-O4 | 2.368(1) | Eu1-O2   | 2.391(1) |          |          |

|     | Eu1-O5 | 2.330(7) | Eu1-O4   | 2.359(7) | Eu1-O7   | 2.477(8) |
|-----|--------|----------|----------|----------|----------|----------|
|     | Eu1-O1 | 2.341(6) | Eu1-O6   | 2.377(5) | Eu1-N5   | 2.649(8) |
|     | Eu1-O3 | 2.348(6) | Eu1-O2   | 2.380(8) |          |          |
|     | Eu2-O10| 2.363(5) | Eu2-O13  | 2.362(4) | Eu2-O14  | 2.401(5) |
|     | Eu2-O11| 2.364(5) | Eu2-O12  | 2.373(4) | Eu2-N3   | 2.642(6) |
|     | Eu2-O9 | 2.369(4) | Eu2-O8   | 2.395(5) |          |          |

Table S5. The C-H⋯π force in 1.

| X-H | d(X-H) (Å) | <DHA(°) | d(X...Cg) (Å) | Cg          |
|-----|------------|---------|----------------|-------------|
| C12-H12 | 0.930     | 118.04  | 3.84(9)       | C9-C10-C11-C12-C13-C14 [1-X,Y, 1/2-Z] |

Table S6. Hydrogen Bonds in 3.

| D-H | d(D-H) (Å) | <DHA(°) | d(D...A) (Å) | A            |
|-----|------------|---------|--------------|--------------|
| O8-H8a | 0.870     | 64.4    | 2.735        | N2 (2-x, 3-y, 2-z) |
| O7-H7  | 0.851     | 171.4   | 2.788        | N6 (1-x,1-y,1-z) |
Figure S6. Powder X-ray diffraction profiles of 1–3 and the simulated ones based on their single crystal structures, all at room temperature.

Figure S7. A comparison of the single-exponential fitting results for observed luminescence decay patterns of complexes 1–4.
2.3 Time-resolved luminescence spectroscopy and transient Mid IR spectroscopy

Figure S8. Transient Mid IR spectroscopy of complexes 1–4 (a–d) varying with different time delay from 0 to 100 ps and their energy relaxation dynamics (e).
3. Computational details

Throughout the manuscript and the supplementary material, the electronic states of the complexes are given as $2S+1(R,M)_n$, where $2S+1$ is the total spin multiplicity of the complex, R and M stand for the labels of the ligand and the Eu$^{3+}$ ion, and n corresponds to the numbering of the electronic states $2S+1(R,M)$ starting from n=0 for the lowest state. It is important to distinguish this numbering of the electronic states of the complexes from the J levels of the Eu$^{3+}$ central ion, although they often take the same values, e.g., the ground state of the complexes is denoted as $7(S_0/F_0)$. Omitting spin-orbit coupling the weak asymmetric ligand field splits $7(S_0/F_0)$ into seven substates $7(S_0/F_n)$ (n=0-6). Using the state interaction approach, matrix elements over the spin-orbit Hamiltonian $\hat{H}_{SO}$ are computed based on these substates and the Hamiltonian matrix is diagonalized resulting in a total of (2S+1)(2L+1)=49 energy levels. Including spin-orbit coupling Eu$^{3+}$ 4$^6$ 7F is split into seven levels $7F_J$ (J=0-6). The corresponding complex substates $7(S_0/F_J)$ are again split due to the ligand field into 2J+1 levels each, yielding again a total of 49 energy levels. Since in the case of the Eu$^{3+}$ complexes considered here spin-orbit interaction is stronger than the ligand field, one may keep the J value as a useful label for the $7(S_0/F_J)_n$ (J=0-6,n=0,1,…49) energy levels of the complexes.

3.1 Model setup: The starting structures for the isolated antennas of PPPD, para-Br-PPPD and meta-Br-PPPD ligand were constructed by density functional theory (DFT) optimization at the B3LYP/6-31G* level. The starting geometries of complexes 1-4 were taken from the crystal structure data by the mechanism-based crystal engineering. The minimum structural units were extracted to undergo further geometry optimizations, which result in the initial structures to describe fully the coordination micro-environment around Eu$^{3+}$ center for the reduction of computational burden of the subsequent high-accurate multi-configurational quantum chemical calculations.

3.2 Complete active space self-consistent field calculations: The complete active space self-consistent field (CASSCF) method$^{51,52}$ has been verified to accurately describe the structural and optical properties of organic systems, transition-metal and lanthanide complexes, especially for those excited states with charge-transfer (CT) character and strong spin-orbit coupling effects.$^{53-57}$ In this work, the ab initio calculations of isolated antennas were primarily performed at the CASSCF level of theory with a total of 12 electrons in 10 active orbitals (12e/10o). In order to describe the CT excitation of the antennas, the high-lying occupied $\pi$ and the low-lying $\pi^*$ orbitals of the diketone, pyridine and benzene ring were included in the active spaces. All orbitals in the active space for the CASSCF(12e/10o) calculations are schematically shown in Figures. S9-11. For the free antennas, 6-31G* basis sets were applied for all atoms.

All minima of the free antennas in their singlet excited states were obtained by full system state-averaged CASSCF optimizations using a two-root equally weighted (0.5:0.5) approach, while a single-root optimization was adopted for the triplet excited states and the ground states. The same state-averaged method was employed to determine the geometry of the intersection space of $S_{CT}$ and $S_0$ state. The minimum-energy crossing points between the $S_{CT}$ and $T_1$ state were optimized using a many-electron basis of Slater determinants. The minimum energy profiles (MEPs) for singlet and triplet relaxation were mapped by intrinsic reaction coordinate (IRC) computations to
connect the above critical points in several possible excited and ground states.\textsuperscript{58,59}

Restricted active space self-consistent field (RASSCF) calculations\textsuperscript{510} were adopted for the complexes 1-4. Three pair of $\pi$ and $\pi^*$ orbitals of the diketone, pyridine and benzene ring were included to describe the involved electron transitions and conjunction effects of the coordinated ligands. Meanwhile, 6 $f$ electrons and their 7 $f$ orbitals (6e/7o) of Eu$^{3+}$ center were added, resulting in a total of 12e/13o active space, to characterize complexes 1-4 in the septet ground state $7(S_0/F)$, and the various excited states, i.e., the quintet $5(S_0/F)$, septet $7(SCT(1\pi\pi^*)/F)$ and nonet $9(3\pi\pi^*/F)$ states. All of these orbitals for the RASSCF(12e/13o) calculations are schematically shown for complexes 1-4 in Figures S12-15.

3.3 Complete active space perturbation theory and relaxation pathways: In order to consider the dynamic electron correlation effects, the single-point energy of the optimized geometries in the above computations was recalculated at the multi-configuration second-order perturbation (CASPT2) level of theory.\textsuperscript{511,512} Five roots state-averaged RASSCF wave functions for the isolated antennas were used as zeroth-order wave function, while different multiple-roots state-averaged RASSCF wave functions for complexes were applied to calculate the energetic levels of the $7(S_0/F)$ (14 roots), $7(1\pi\pi^*/F)$ (14 roots), $9(3\pi\pi^*/F)$ (14/7 roots), and $5(S_0/F)$ (5 roots) states and their splitting in corresponding sublevels. As a result, the minimum energy profiles of free antennas and the chelated complexes were eventually computed at the CASPT2//IRC/CASSCF level of theory along the unbiased reaction coordinates to obtain the relaxation path of isolate ligands and the radiative-EnT pathways of lanthanide complexes 1-4 elucidating their photoluminescence mechanisms. The vertical excitation energies and the corresponding oscillator strengths ($f$) for the different transitions of the ligands and complexes were calculated by 4 or 3 roots state-averaged CASSCF state interaction (CASSI) computations at their corresponding ground state geometries.

3.4 Spin-orbit coupling calculations and kinetic assessment on the ligand-centered ISC: The SO matrix elements between the involved states for the complexes 1-4 were computed by using the pseudopotential spin-orbit operator on Eu$^{3+}$ and the Breit-Pauli operator on all other atoms.\textsuperscript{513,514} For the quintet-septet couplings, the active space of six $f$ electrons in seven $f$ orbitals, i.e. (6e/7o), was adopted to compute the $5(S_0/F_J,J=0-4, n=0,1,...,25)$ and the $7(S_0/F_J,J=0-6, n=0,1,...,49)$ couplings, which results in a total of 74×74 = 5476 matrix elements. While for the septet-nonet couplings, the targeted pair of antenna $\pi/\pi^*$ was added with a total (8e/9o) space to judge the efficiency of intersystem crossing for the complexes. The SO matrix elements number for septet-nonet couplings, i.e., $7(S_0/F_J,J=0-6, n=0,1,...,98)$ and $9(3\pi\pi^*/F_J,J=0-6, n=0,1,...,63)$, is 161×161 = 25921. It should be noted that for the effective one-electron Eu spin-orbit operator used in this work there is no direct coupling of the nonet $9(3\pi\pi^*/F)$ and quintet $5(S_0/F)$ states in the spin-orbit Hamiltonian matrix, but rather an indirect coupling mediated by septet states. These values were afterwards used in the spin–orbit coupling matrices to calculate subsequently eigenstates and properties, within a many-electron basis set consisting of spin-free electronic states of the CASSCF or RASSCF calculations. The ligand-centered ISC rate $k_{ISC}$ from the initial state I to final state F was evaluated in the Condon
approximation as follows,

\[ k_{\text{ISC}} = \frac{2\pi}{\hbar} \langle 1\psi_0 | H_{\text{SO}} | 3\psi_0^F \rangle^2 \langle \chi_0 | \chi_n >^2 \rho \]

where \( H_{\text{SO}} \) indicates spin-orbit coupling vector between initial \( I \) to final \( F \) state. The Franck−Condon factor \( \langle \chi_0 | \chi_n > \) was taken equal to 1 and \( \rho = 1/\Delta E_{IF} \).

The rate constants of radiative/nonradiative relaxations \( (k_{\text{rad}}/k_{\text{nr}}, \text{s}^{-1}) \) and the metal radiative decay efficiencies \( (\eta_{\text{Eu}}) \) were calculated based on the experimentally recorded overall quantum yields \( (\Phi_{\text{QY}}) \) and lifetimes \( (\tau) \) using the formula below.

\[ k_{\text{rad}} = 1 / \tau_{\text{rad}} = A_{\text{MD}} \cdot n^3 \cdot I_{\text{tot}}/I_{\text{MD}} \]

\[ k_{\text{nr}} = k_{\text{obs}} - k_{\text{rad}} = 1 / \tau_{\text{obs}} - 1 / \tau_{\text{rad}} \]

\[ \eta_{\text{Eu}} = \tau_{\text{obs}} / \tau_{\text{rad}} = k_{\text{rad}} / k_{\text{obs}} \]

where \( I_{\text{tot}} \) is the integrated emission intensity over all of the \( ^5D_0 \rightarrow ^7F_J \) transitions and \( I_{\text{MD}} \) is the integrated intensity of the \( ^5D_0 \rightarrow ^7F_1 \) transition (measured from 580–600 nm). \( A_{\text{MD}} \), represents the spontaneous emission probability of the \( ^5D_0 \rightarrow ^7F_1 \) transition, with a value of 14.65 s\(^{-1}\) in vacuo, \( n \) is the refractive index (1.51).
3.5 References

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3.6 Selected orbitals in the active space

Plots of selected orbitals in the active spaces for the free antennas PPPD, \textit{para}-Br-PPPDD and \textit{meta}-Br-PPPDD anion and their corresponding complexes 1-4. The subscripts reflect the main character of the orbitals.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{image}
\caption{Molecular orbitals of PPPD used in defining the active space for the CASPT2//CASSCF(12e/10o) calculations.}
\end{figure}
Figure S10. Molecular orbitals of para-Br-PPPD used in defining the active space for the CASPT2/CASSCF(12e/10o) calculations.

Figure S11. Molecular orbitals of meta-Br-PPPD used in defining the active space for the CASPT2/CASSCF(12e/10o) calculations.
Figure S12. Molecular orbitals of complex 1 used in defining the active space for the CASPT2//RASSCF(12e/13o) calculations.
Figure S13. Molecular orbitals of complex 2 used in defining the active space for the CASPT2//RASSCF(12e/13o) calculations.
Figure S14. Molecular orbitals of complex 3 used in defining the active space for the CASPT2//RASSCF(12e/13o) calculations.
Figure S15. Molecular orbitals of complex 4 used in defining the active space for the CASPT2/RASSCF(12e/13o) calculations.
3.7 Optimized structures

**Figure S16.** The critical structures of PPPD obtained at the CASSCF(12e/10o) level of theory. Selected key bond lengths are given in angstrom (Å) (see Sect. 3.9 for Cartesian coordinates).
Figure S17. The critical structures of para-Br-PPPD obtained at the CASSCF(12e/10o) level of theory. Selected key bond lengths are given in angstrom (Å) (see Sect. 3.9 for Cartesian coordinates).
Figure S18. The critical structures of meta-Br-PPPD obtained at the CASSCF(12e/10o) level of theory. Selected key bond lengths are given in angstrom (Å) (see Sect. 3.9 for Cartesian coordinates).
**Figure S19.** The critical structures of complex 1 obtained at the CASSCF(12e/13o) level of theory. Hydrogen atoms are omitted for clarity. Selected key bond lengths are given in angstrom (Å). (see Sect. 3.9 for Cartesian coordinates).
**Figure S20.** The critical structures of complex 2 obtained at the CASSCF(12e/13o) level of theory. Hydrogen atoms are omitted for clarity. Selected key bond lengths are given in angstrom (Å). (see Sect. 3.9 for full Cartesian coordinates).
Figure S21. The critical structures of complex 3 obtained at the CASSCF(12e/13o) level of theory. Hydrogen atoms are omitted for clarity. Selected key bond lengths are given in angstrom (Å). (see Sect. 3.9 for full Cartesian coordinates).
Figure S22. The critical structures of complex 4 obtained at the CASSCF(12e/13o) level of theory. Hydrogen atoms are omitted for clarity. Selected key bond lengths are given in angstrom (Å). (see Sect. 3.9 for full Cartesian coordinates).
### 3.8 Energy tables

**Table S7.** Vertical excitation energies ($E_{\perp}$, kcal mol$^{-1}$), oscillator strengths ($f$), dipole moments ($\Delta \text{D.M.}$, Debye), and singly occupied orbitals in the $S_0 \rightarrow S_1(\text{11}\pi\pi^*)$ electronic transitions of the antennas PPPD, para-Br-PPPD and meta-Br-PPPD formed complexes 1–4.

| Transition | D.M. | f   | $\Delta E$ | singly occupied orbitals |
|------------|------|-----|-----------|--------------------------|
| $S_0$      | 8.6  | --  | 0.0       |                          |
| **Complex 1** |     |     |           |                          |
| $^\gamma(S_0/\gamma F_0 \rightarrow S_1(\text{11}\pi\pi^*)/\gamma F_0)$ | 3.4 | 0.53 | 61.8 | $\pi\pi^*$–dione |
| $S_0$      | 5.9  | --  | 0.0       |                          |
| **Complex 3** |     |     |           |                          |
| $^\gamma(S_0/\gamma F_0 \rightarrow S_1(\text{11}\pi\pi^*)/\gamma F_0)$ | 5.6 | 0.79 | 62.9 | $\pi\pi^*$–dione |
| $S_0$      | 12.5 | --  | 0.0       |                          |
| **Complex 4** |     |     |           |                          |
| $^\gamma(S_0/\gamma F_0 \rightarrow S_1(\text{11}\pi\pi^*)/\gamma F_0)$ | 12.2 | 0.57 | 62.3 | $\pi\pi^*$–dione |


| Critical points | Transitions | SOME/cm⁻¹ |
|----------------|-------------|------------|
|                |             | ligand     | metal     |
| 7(S(1′ππ′)/7F₀)−Min | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₀ | 0.3−1.8    |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₁ | 36−317     |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₂ | 7−157      |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₃ | 17−183     |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₄ | 5−99       |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₅ | 1.4−7.5    |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₆ | 2−87       |
| 9(3ππ⁴)/F₀−Min | 9(3ππ⁴)/F₀→ 9(3ππ⁴)/F₁ | 332−1454   |
| 5(S₀⁶/D₀)−Min  | 5(S₀⁶/D₀)→ 7(S₀⁷/F₀) | 9−349      |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₁) | 24−1580    |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₂) | 433−1679   |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₃) | 69−799     |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₄) | 148−1037   |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₅) | 85−440     |
|                | 5(S₀⁶/D₀)→ 7(S₀⁷/F₆) | 4−555      |
|                | 5(S₀⁶/D₀)→ 5(S₀⁶/D₁) | 34−657     |
|                | 9(3ππ⁴)/F₀→ 5(S₀⁶/D₁) | 412−1597   |
|                | 5(S₀⁶/D₀)→ 5(S₀⁶/D₁) | 559−1118   |
| 7(S₁(1′ππ′)/7F₀)−Min | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₀ | 0.5−2.8    |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₁ | 54−287     |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₂ | 19−101     |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₃ | 14−191     |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₄ | 9−148      |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₅ | 6−84       |
|                | 7(1′ππ′)/F₀→ 9(3ππ⁴)/F₆ | 17−102     |
| Complex 4 | \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_0)\) | 0.3–2.2 | 35–969 |
|----------|---------------------------------|--------|--------|
|          | \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_1)\) |        | 271–1536 |
|          | \(^5(S_0/F_0)\rightarrow 5(S_0/F_1)\) |        | 884–2594 |

| \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_0)\) | 0.3-1.9 | 77-298 |
| \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_1)\) |        | 373-1444 |
| \(^5(S_0/F_0)\rightarrow 5(S_0/F_1)\) |        | 418-921 |

| \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_0)\) | 28-686 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_0)\) |        | 219-1196 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_2)\) |        | 351-1358 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_3)\) |        | 239-926 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_4)\) |        | 53-1117 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_6)\) |        | 130-909 |
| \(^5(S_0/F_0)\rightarrow 7(S_0/F_6)\) |        | 122-618 |

| \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_0)\) | 171-783 |
| \(^9(3\pi\pi^*/F_0)\rightarrow 5(S_0/F_1)\) |        | 37-199 |
| \(^5(S_0/F_0)\rightarrow 5(S_0/F_1)\) |        | 337-1444 |
| \(^5(S_0/F_0)\rightarrow 5(S_0/F_1)\) |        | 418-921 |
Table S9. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol\(^{-1}\)) with respect to their corresponding ground state \(\gamma(S_0/F_0)\) for the optimized structures of the complexes 1-4 in the energy resonant region (nonet-quintet crossing, NQC) obtained at the CASPT2 level. The corresponding energy profiles are plotted in Figure 3 of the main article.

| NQC | \(\gamma(3\pi\pi^*/F)\) | RASSCF | CASPT2 |
|-----|-----------------|--------|--------|
|     | A.E.            | A.E.   | R.E.   |
| \(7(S_0/F)\)\(_{e=6}\) |                  |        |        |
| Root1 \(\gamma(S_0/F_0)\) | -3398.172186    | -3404.72011 | 0.0   |
| Root2 | -3398.171434    |        |        |
| Root3 | -3398.168223    |        |        |
| Root4 | -3398.167555    |        |        |
| Root5 | -3398.167287    |        |        |
| Root6 | -3398.166461    |        |        |
| Root7 | -3398.165528    |        |        |
| \(\gamma(S_0^*/F)\)\(_{e=6}\) |                  |        |        |
| Root1 \(\gamma(S_0^*/F_0)\) | -3398.174723    | -3404.706365 | 8.6   |
| Root2 | -3398.173948    |        |        |
| Root3 | -3398.170734    |        |        |
| Root4 | -3398.170117    |        |        |
| Root5 | -3398.169799    |        |        |
| Root6 | -3398.168752    |        |        |
| Root7 | -3398.168207    |        |        |
| \(\gamma(3\pi\pi^*/F)\)\(_{e=6}\) |                  |        |        |
| Root1 \(\gamma(3\pi\pi^*/F_0)\) | -3398.043138    | -3404.62221 | 61.4 (541 nm) |
| Root2 | -3398.042403    |        |        |
| Root3 | -3398.039226    |        |        |
| Root4 | -3398.038615    |        |        |
| Root5 | -3398.038467    |        |        |
| Root6 | -3398.037254    |        |        |
| Root7 | -3398.036713    |        |        |
| \(\pi(S_0^D)\)\(_{e=4}\) |                  |        |        |
| Root1 \(\pi(S_0^D_0)\) | -3398.045158    | -3404.62640 | 58.8 (570 nm) |
| Root2 | -3398.043851    |        |        |
| Root3 | -3398.040383    |        |        |
| Root4 | -3398.038410    |        |        |
| Root5 \(\pi(S_0^D_1)\) | -3398.037824    | -3404.62038 | 62.6 (530 nm) |

Complex 1

Complex 2

| NQC | \(\gamma(S_0/F)\) | RASSCF | CASPT2 |
|-----|-----------------|--------|--------|
|     | A.E.            | A.E.   | R.E.   |
| \(7(S_0/F)\)\(_{e=6}\) |                  |        |        |
| Root1 \(\gamma(S_0/F_0)\) | -3435.882186    | -3442.86077 | 0.0   |
| Root2 | -3435.880913    |        |        |
| Root3 | -3435.877958    |        |        |
| Root4 | -3435.877228    |        |        |
| Root5 | -3435.876999    |        |        |
| Root6 | -3435.876258    |        |        |
| Complex 3 |  |
|---|---|
| $^1\text{S}_0^*/\text{F}$ |  |
| Root1 | $^1\text{S}_0^*/\text{F}_0$ | -3435.867738 | -3442.84699 | 8.7 |
| Root2 | -3435.866433 |  |
| Root3 | -3435.863435 |  |
| Root4 | -3435.862714 |  |
| Root5 | -3435.862484 |  |
| Root6 | -3435.861583 |  |
| Root7 | -3435.861138 |  |

| $^3\text{S}_0^*/\text{F}$ |  |
|---|---|
| Root1 | $^3\text{S}_0^*/\text{F}_0$ | -3435.770193 | -3442.76528 | 59.9 (558 nm) |
| Root2 | -3435.768927 |  |
| Root3 | -3435.765940 |  |
| Root4 | -3435.765274 |  |
| Root5 | -3435.765011 |  |
| Root6 | -3435.764033 |  |
| Root7 | -3435.763552 |  |

| $^5\text{S}_0^*/\text{D}$ |  |
|---|---|
| Root1 | $^5\text{S}_0^*/\text{D}_0$ | -3435.772178 | -3442.76560 | 59.7 (560 nm) |
| Root2 | -3435.770409 |  |
| Root3 | -3435.767016 |  |
| Root4 | -3435.765018 |  |
| Root5 | -3435.764421 | -3442.75943 | 63.6 (520 nm) |

| $^1\text{S}_0^*/\text{F}$ |  |
|---|---|
| Root1 | $^1\text{S}_0^*/\text{F}_0$ | -3267.275103 | -3273.94426 | 0.0 |
| Root2 | -3267.274130 |  |
| Root3 | -3267.272940 |  |
| Root4 | -3267.271885 |  |
| Root5 | -3267.271279 |  |
| Root6 | -3267.270984 |  |
| Root7 | -3267.270938 |  |

| $^3\text{S}_0^*/\text{F}$ |  |
|---|---|
| Root1 | $^3\text{S}_0^*/\text{F}_0$ | -3267.265009 | -3273.94169 | 1.6 |
| Root2 | -3267.263941 |  |
| Root3 | -3267.262884 |  |
| Root4 | -3267.261858 |  |
| Root5 | -3267.261235 |  |
| Root6 | -3267.260892 |  |
| Root7 | -3267.260866 |  |

| $^3\text{S}_0^*/\text{D}$ |  |
|---|---|
| Root1 | $^3\text{S}_0^*/\text{D}_0$ | -3267.158481 | -3273.85698 | 54.8 (538 nm) |
| Root2 | -3267.157425 |  |
| Root3 | -3267.156475 |  |
| Complex 4 | Root4 | -3267.155430 |
| Complex 4 | Root5 | -3267.154705 |
| Complex 4 | Root6 | -3267.154579 |
| Complex 4 | Root7 | -3267.154338 |
| $^5(S_0^0D)_0$ $^2$ | Root1  | $^5(S_0^0D_0)$ | -3267.162129 | -3273.86299 | 51.0 (579 nm) |
| $^5(S_0^0D)_0$ $^2$ | Root2  | -3267.161995 |
| $^5(S_0^0D)_0$ $^2$ | Root3  | -3267.161780 |
| $^5(S_0^0D)_0$ $^2$ | Root4  | -3267.161474 |
| $^5(S_0^0D)_0$ $^2$ | Root5  | $^5(S_0^0D_1)$ | -3267.161279 | -3273.85777 | 54.3 (543 nm) |

| 7(S_0/F) 0-6  | Root1  | $^7(S_0^0F_0)$ | -3583.534879 | -3590.60478 | 0.0 |
| 7(S_0/F) 0-6  | Root2  | -3583.534015 |
| 7(S_0/F) 0-6  | Root3  | -3583.532419 |
| 7(S_0/F) 0-6  | Root4  | -3583.532169 |
| 7(S_0/F) 0-6  | Root5  | -3583.531853 |
| 7(S_0/F) 0-6  | Root6  | -3583.531793 |
| 7(S_0/F) 0-6  | Root7  | -3583.531329 |

| $^7(S_0^*/F_0)$ 0-6  | Root1  | $^7(S_0^*/F_0)$ | -3583.521675 | -3590.60436 | 0.3 |
| $^7(S_0^*/F_0)$ 0-6  | Root2  | -3583.520773 |
| $^7(S_0^*/F_0)$ 0-6  | Root3  | -3583.519156 |
| $^7(S_0^*/F_0)$ 0-6  | Root4  | -3583.518819 |
| $^7(S_0^*/F_0)$ 0-6  | Root5  | -3583.518517 |
| $^7(S_0^*/F_0)$ 0-6  | Root6  | -3583.518344 |
| $^7(S_0^*/F_0)$ 0-6  | Root7  | -3583.517921 |

| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root1  | $^9(3\pi^0\pi^*/F_0)$ | -3583.410487 | -3590.527226 | 48.7 (590 nm) |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root2  | -3583.409552 |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root3  | -3583.407933 |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root4  | -3583.407632 |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root5  | -3583.407356 |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root6  | -3583.407012 |
| $^9(3\pi^0\pi^*/F_0)$ 0-6 | Root7  | -3583.406524 |

| $^5(S_0^0D)_0$ 0-4 | Root1  | $^5(S_0^0D_0)$ | -3583.409221 | -3590.527588 | 48.4 (593 nm) |
| $^5(S_0^0D)_0$ 0-4 | Root2  | -3583.408981 |
| $^5(S_0^0D)_0$ 0-4 | Root3  | -3583.408916 |
| $^5(S_0^0D)_0$ 0-4 | Root4  | -3583.408614 |
| $^5(S_0^0D)_0$ 0-4 | Root5  | $^5(S_0^0D_1)$ | -3583.408544 | -3590.52188 | 52.0 (552 nm) |
Table S10. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol\(^{-1}\)) for PPPD along the relaxation pathway in S\(_{CT}(^1\pi\pi^*)\) and T\(_1(3\pi\pi^*)\) state. The corresponding ground state energy is also given. The minimum energy profiles have been plotted in Figure S1.

|                  | RASSCF A.E. | RASCC A.E. | CASPT2 R.E. |
|------------------|-------------|-------------|--------------|
| **S\(_0\)-Min** |             |             |              |
| Root1(S\(_0\))  | -740.219390 | -742.40646  | 0.0          |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.077612 | -742.28977  | 73.2         |
| **Path-S\(_{CT}(^1\pi\pi^*)\)-1** |             |             |              |
| Root1(S\(_0\))  | -740.217367 | -742.40597  | 0.3          |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.085705 | -742.29684  | 68.8         |
| **S\(_{CT}(^1\pi\pi^*)\)-Min** |             |             |              |
| Root1(S\(_0\))  | -740.197584 | -742.39000  | 10.3         |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.097120 | -742.30377  | 64.4         |
| **Path-S\(_{CT}(^1\pi\pi^*)\)-4** |             |             |              |
| Root1(S\(_0\))  | -740.191738 | -742.38509  | 13.4         |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.097917 | -742.30300  | 64.9         |
| **Path-S\(_{CT}(^1\pi\pi^*)\)-5** |             |             |              |
| Root1(S\(_0\))  | -740.189030 | -742.38252  | 15.0         |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.097623 | -742.30235  | 65.3         |
| **Path-S\(_{CT}(^1\pi\pi^*)\)-6** |             |             |              |
| Root1(S\(_0\))  | -740.186990 | -742.38110  | 15.9         |
| Root2[S\(_{CT}(^1\pi\pi^*)\)] | -740.097508 | -742.30247  | 65.3         |
| Path−S_{CT}(\pi\pi^*)−8 |  |  |
|--------------------------|---|---|
| Root1(S_0)               | -740.190506 | -742.38376 | 14.2 |
| Root2 [S_{CT}(\pi\pi^*)] | -740.097631 | -742.30246 | 65.3 |

| Path−S_{CT}(\pi\pi^*)−9 |  |  |
|--------------------------|---|---|
| Root1(S_0)               | -740.193186 | -742.38495 | 13.5 |
| Root2 [S_{CT}(\pi\pi^*)] | -740.097835 | -742.30317 | 65.3 |

| Path−S_{CT}(\pi\pi^*)−10 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.193734 | -742.385113 | 13.4 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.097602 | -742.303107 | 64.9 |

| Path−S_{CT}(\pi\pi^*)−11 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.193863 | -742.385063 | 13.4 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.097382 | -742.303130 | 64.8 |

| Path−S_{CT}(\pi\pi^*)−12 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.193651 | -742.384790 | 13.6 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.097155 | -742.303137 | 64.8 |

| Path−S_{CT}(\pi\pi^*)−13 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.193193 | -742.384548 | 13.7 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.097028 | -742.303377 | 64.7 |

| Path−S_{CT}(\pi\pi^*)−14 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.199945 | -742.382255 | 15.2 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.098882 | -742.302361 | 65.3 |

| Path−S_{CT}(\pi\pi^*)−15 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.198597 | -742.378928 | 17.3 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.091829 | -742.303591 | 64.6 |

| Path−S_{CT}(\pi\pi^*)−16 |  |  |
|---------------------------|---|---|
| Root1(S_0)                | -740.195611 | -742.374572 | 20.0 |
| Root2 [S_{CT}(\pi\pi^*)]  | -740.090340 | -742.302554 | 65.2 |
| Path−$S_{CT}(^1\pi\pi')$−17 | Root1($S_0$) | $-740.191594$ | $-742.368878$ | 23.6 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.089276$ | $-742.301794$ | 65.7 |
| Path−$S_{CT}(^1\pi\pi')$−18 | Root1($S_0$) | $-740.193267$ | $-742.370878$ | 22.3 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.092979$ | $-742.311343$ | 63.0 |
| Path−$S_{CT}(^1\pi\pi')$−19 | Root1($S_0$) | $-740.194693$ | $-742.372795$ | 21.1 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.097370$ | $-742.311343$ | 59.7 |
| Path−$S_{CT}(^1\pi\pi')$−20 | Root1($S_0$) | $-740.136014$ | $-742.344337$ | 39.0 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.132431$ | $-742.312374$ | 59.0 |
| STC( $S_{CT}/T_1$) | Root1($S_0$) | $-740.136717$ | $-742.343409$ | 39.6 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.132826$ | $-742.315826$ | 56.9 |
| Path−$S_{CT}(^1\pi\pi')$−22 | Root1($S_0$) | $-740.137325$ | $-742.342588$ | 40.1 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.133132$ | $-742.318437$ | 55.2 |
| Path−$S_{CT}(^1\pi\pi')$−23 | Root1($S_0$) | $-740.137800$ | $-742.341972$ | 40.5 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.133419$ | $-742.320552$ | 53.9 |
| CI( $S_{CT}/S_0$) | Root1($S_0$) | $-740.129804$ | $-742.327095$ | 49.8 |
| Root2 [$S_{CT}(^1\pi\pi')$] | $-740.126573$ | $-742.321118$ | 53.6 |
| Path−$T_1(^2\pi\pi')$−1 | Root1[$T_1(^2\pi\pi')$] | $-740.095777$ | $-742.316326$ | 56.6 |
| Path−T₁(3ππ')−2 | Root₁[T₁(3ππ')] | -740.106141 | -742.320309 | 54.1 |
|------------------|------------------|-------------|-------------|-----|
| Path−T₁(3ππ')−3 | Root₁[T₁(3ππ')] | -740.107934 | -742.322661 | 52.6 |
| Path−T₁(3ππ')−4 | Root₁[T₁(3ππ')] | -740.095414 | -742.323701 | 51.9 |
| T₁(3ππ')−Min    | Root₁[T₁(3ππ')] | -740.103032 | -742.329578 | 48.2 |
Table S11. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol\(^{-1}\)) for para-Br-PPPD along the relaxation pathway in \(S_{\text{CT}}(1\pi\pi^*)\) and \(T_1(3\pi\pi^*)\) state. The corresponding ground state energy is also given. The minimum energy profiles have been plotted in Figure S1.

|        | RASSCF          | CASPT2          |
|--------|-----------------|-----------------|
|        | A.E.            | A.E.            | R.E.  |
| \(S_0\) |                 |                 |       |
| Root1 \((S_0)\) | -752.774409 | -755.10244 | 0.00  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.635555 | -754.98985 | 70.7  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-1 |   |                 |       |
| Root1 \((S_0)\) | -752.772899 | -755.10153 | 0.6   |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.645085 | -754.99681 | 66.3  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-2 |   |                 |       |
| Root1 \((S_0)\) | -752.765899 | -755.09560 | 4.3   |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.653937 | -755.00263 | 62.6  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-3 |   |                 |       |
| Root1 \((S_0)\) | -752.753698 | -755.08449 | 11.3  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.657211 | -755.00376 | 61.9  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-4 |   |                 |       |
| Root1 \((S_0)\) | -752.751712 | -755.08279 | 12.3  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.658358 | -755.00395 | 61.8  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-5 |   |                 |       |
| Root1 \((S_0)\) | -752.749751 | -755.08122 | 13.3  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.658503 | -755.00384 | 61.9  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-6 |   |                 |       |
| Root1 \((S_0)\) | -752.750324 | -755.08158 | 13.1  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.658384 | -755.00383 | 61.9  |
| Path\(-S_{\text{CT}}(1\pi\pi^*)\)-7 |   |                 |       |
| Root1 \((S_0)\) | -752.747967 | -755.07975 | 14.2  |
| Root2 [\(S_{\text{CT}}(1\pi\pi^*)\)] | -752.658261 | -755.00374 | 61.9  |
| Path  | $\text{S}_{CT}(\pi\pi')$-8 |     |     |    |
|-------|--------------------------|-----|-----|----|
| Root1($S_0$) | -752.747386 | -755.07957 | 14.4 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658136 | -755.00395 | 61.8 |

| Path  | $\text{S}_{CT}(\pi\pi')$-9 |
|-------|--------------------------|
| Root1($S_0$) | -752.746973 | -755.07911 | 14.6 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658402 | -755.00364 | 61.8 |

| Path  | $\text{S}_{CT}(\pi\pi')$-10 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.747312 | -755.07940 | 14.6 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658153 | -755.00386 | 61.9 |

| Path  | $\text{S}_{CT}(\pi\pi')$-11 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.747361 | -755.07946 | 14.4 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658116 | -755.00387 | 61.9 |

| Path  | $\text{S}_{CT}(\pi\pi')$-12 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.747884 | -755.07981 | 14.2 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.657514 | -755.00335 | 62.2 |

| Path  | $\text{S}_{CT}(\pi\pi')$-13 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.747934 | -755.07997 | 14.1 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658076 | -755.00380 | 61.9 |

| Path  | $\text{S}_{CT}(\pi\pi')$-14 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.747388 | -755.07942 | 14.4 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658273 | -755.00384 | 61.9 |

| Path  | $\text{S}_{CT}(\pi\pi')$-15 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.746823 | -755.07891 | 14.8 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.658542 | -755.00389 | 61.8 |

| Path  | $\text{S}_{CT}(\pi\pi')$-16 |     |     |    |
|-------|-----------------------------|-----|-----|----|
| Root1($S_0$) | -752.745208 | -755.07751 | 15.6 |
| Root2 [$S_{CT}(\pi\pi')$] | -752.659162 | -755.00402 | 61.8 |
| Path–S<sub>CT(ππ')</sub>–17 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.763311 | -755.07568 | 16.8 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.662832 | -755.00690 | 60.0 |

| Path–S<sub>CT(ππ')</sub>–18 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.762518 | -755.07511 | 17.2 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.663646 | -755.00763 | 59.5 |

| Path–S<sub>CT(ππ')</sub>–19 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.740625 | -755.07476 | 17.4 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.664031 | -755.01124 | 58.5 |

| Path–S<sub>CT(ππ')</sub>–20 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.737269 | -755.07238 | 18.9 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.665993 | -755.01124 | 57.2 |

| Path–S<sub>CT(ππ')</sub>–21 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.735553 | -755.07112 | 19.6 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.667073 | -755.01202 | 56.7 |

| S<sub>CT(ππ')</sub>–Min/STC(S₁/T₁) |         |         |     |
|------------------------------------|---------|---------|-----|
| Root1(S₀)                          | -752.758081 | -755.05558 | 29.4 |
| Root2[S<sub>CT(ππ')</sub>]        | -752.701186 | -755.01780 | 53.1 |
| Root1[T₁(³ππ')]                   | -752.672899 | -755.01797 | 53.0 |

| Path–S<sub>CT(ππ')</sub>–23 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1                         | -752.733426 | -755.04982 | 33.0 |
| Root2                         | -752.677971 | -755.01602 | 54.2 |

| Path–S<sub>CT(ππ')</sub>–24 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.723932 | -755.04356 | 36.9 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.677195 | -755.01422 | 55.4 |

| Path–S<sub>CT(ππ')</sub>–25 |         |         |     |
|------------------------------|---------|---------|-----|
| Root1(S₀)                    | -752.683958 | -755.02582 | 48.1 |
| Root2[S<sub>CT(ππ')</sub>]  | -752.675327 | -755.01327 | 56.0 |
| CI($S_{CT}/S_0$) |       |       |
|------------------|-------|-------|
| Root1($S_0$)     | -752.662018 | -755.00295 | 62.4 |
| Root2[$S_{CT}(1\pi\pi')$] | -752.652155 | -754.99734 | 66.0 |
| Path–$T_1(3\pi\pi')$–1 |       |       |
| Root1[$T_1(3\pi\pi')$] | -752.673463 | -755.01621 | 54.1 |
| Path–$T_1(3\pi\pi')$–2 |       |       |
| Root1[$T_1(3\pi\pi')$] | -752.671521 | -755.01424 | 55.3 |
| Path–$T_1(3\pi\pi')$–3 |       |       |
| Root1[$T_1(3\pi\pi')$] | -752.672098 | -755.01542 | 54.6 |
| $T_1(3\pi\pi')$–Min |       |       |
| Root1[$T_1(3\pi\pi')$] | -752.672319 | -755.01791 | 53.0 |
Table S12. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol$^{-1}$) for meta-Br-PPPD along the relaxation pathway in $S_{CT}(1\pi\pi^*)$ and $T_1(3\pi\pi^*)$ state. The corresponding ground state energy is also given. The minimum energy profiles have been plotted in Figure S1.

| Path |  | RASSCF | CASPT2 |
|------|----------------|--------|---------|
|      | A.E. | A.E.  | R.E.   |
| $S_0$ |      |        |        |
| Root1($S_0$) | $-752.771747$ | $-755.10032$ | $0.00$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.633401$ | $-754.98759$ | $70.7$ |
| Path $-S_{CT}(1\pi\pi^*)-1$ | | | |
| Root1($S_0$) | $-752.771536$ | $-755.10027$ | $0.1$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.638583$ | $-754.99145$ | $68.3$ |
| Path $-S_{CT}(1\pi\pi^*)-2$ | | | |
| Root1($S_0$) | $-752.770612$ | $-755.09949$ | $0.5$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.643138$ | $-754.99466$ | $66.3$ |
| Path $-S_{CT}(1\pi\pi^*)-3$ | | | |
| Root1($S_0$) | $-752.768370$ | $-755.09723$ | $1.9$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.648409$ | $-754.99781$ | $64.3$ |
| Path $-S_{CT}(1\pi\pi^*)-4$ | | | |
| Root1($S_0$) | $-752.765939$ | $-755.09503$ | $3.3$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.651404$ | $-754.99974$ | $63.1$ |
| Path $-S_{CT}(1\pi\pi^*)-5$ | | | |
| Root1($S_0$) | $-752.762874$ | $-755.09229$ | $5.0$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.653740$ | $-755.00109$ | $62.3$ |
| Path $-S_{CT}(1\pi\pi^*)-6$ | | | |
| Root1($S_0$) | $-752.758186$ | $-755.08800$ | $7.7$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.655935$ | $-755.00198$ | $61.7$ |
| Path $-S_{CT}(1\pi\pi^*)-7$ | | | |
| Root1($S_0$) | $-752.752110$ | $-755.08262$ | $11.1$ |
| Root2 [$S_{CT}(1\pi\pi^*)$] | $-752.657156$ | $-755.00233$ | $61.5$ |
| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.745906 | -755.07744 | 14.4 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.657955 | -755.00256 | 61.3 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.745616 | -755.07733 | 14.4 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.658362 | -755.00299 | 61.3 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.744845 | -755.07698 | 14.6 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.659472 | -755.00410 | 60.4 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.744319 | -755.07672 | 14.8 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.660146 | -755.00477 | 60.0 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.743671 | -755.07634 | 15.0 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.660867 | -755.00545 | 59.5 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.742954 | -755.07593 | 15.3 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.661635 | -755.00618 | 59.1 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.742137 | -755.07547 | 15.6 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.662433 | -755.00695 | 58.6 |

| Path $\text{S}_{\text{CT}}(\pi\pi^*)$ |  |  |
|---|---|---|
| Root1($S_0$) | -752.741188 | -755.07485 | 16.0 |
| Root2 [S_{\text{CT}}(\pi\pi^*)] | -752.663260 | -755.00772 | 58.1 |
| Path−$S_{CT}(\pi^\pi^\ast)$−17 |   |   |   |
|-------------------------|---|---|---|
| Root1($S_0$)            | -752.740343 | -755.07454 | 16.2 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.663924 | -755.00868 | 57.5 |

| Path−$S_{CT}(\pi^\pi^\ast)$−18 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.739315 | -755.07368 | 16.7 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.664711 | -755.00921 | 57.5 |

| Path−$S_{CT}(\pi^\pi^\ast)$−19 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.737096 | -755.07218 | 17.7 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.666127 | -755.01069 | 56.2 |

| Path−$S_{CT}(\pi^\pi^\ast)$−20 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.735906 | -755.07125 | 18.2 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.667089 | -755.01133 | 55.8 |

| Path−$S_{CT}(\pi^\pi^\ast)$−21 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.734533 | -755.07020 | 18.9 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.667906 | -755.01198 | 55.4 |

| Path−$S_{CT}(\pi^\pi^\ast)$−22 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.733460 | -755.06945 | 19.4 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.668519 | -755.01259 | 55.1 |

| Path−$S_{CT}(\pi^\pi^\ast)$−23 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.732510 | -755.06876 | 19.8 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.668869 | -755.01296 | 54.8 |

| $S_{CT}(\pi^\pi^\ast)$−Min / STC ($S_1/T_1$) |   |   |   |
|------------------|---|---|---|
| Root1($S_0$)     | -752.731441 | -755.06791 | 20.3 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.669481 | -755.01345 | 54.5 |
| Root1($T_1(2\pi^\pi^\ast)$) | -752.675123 | -755.01731 | 52.1 |

| Path−$S_{CT}(\pi^\pi^\ast)$−25 |   |   |   |
|----------------------|---|---|---|
| Root1($S_0$)         | -752.752287 | -755.06013 | 25.2 |
| Root2[$S_{CT}(\pi^\pi^\ast)$] | -752.678711 | -755.00820 | 57.8 |
| Path $- S_{CT}(1\pi\pi^*)$ | 26 |
|-----------------------------|----|
| Root1($S_0$) | -752.731478 | -755.04213 | 36.5 |
| Root2[$S_{CT}(1\pi\pi^*)]$ | -752.671678 | -755.00092 | 62.4 |

| Path $- S_{CT}(1\pi\pi^*)$ | 27 |
|-----------------------------|----|
| Root1($S_0$) | -752.672663 | -754.98988 | 69.2 |
| Root2[$S_{CT}(1\pi\pi^*)]$ | -752.654809 | -754.98391 | 73.0 |

| CI($S_{CT}/S_0$) |
|------------------|
| Root1($S_0$) | -752.667339 | -754.98433 | 72.8 |
| Root2[$S_{CT}(1\pi\pi^*)$] | -752.652163 | -754.98246 | 74.0 |

| Path $- T_1(3\pi\pi^*)$ | 1 |
|---------------------------|----|
| Root1[$T_1(3\pi\pi^*)$] | -752.674743 | -755.01662 | 52.5 |

| Path $- T_1(3\pi\pi^*)$ | 2 |
|---------------------------|----|
| Root1[$T_1(3\pi\pi^*)$] | -752.671485 | -755.01306 | 54.8 |

| Path $- T_1(3\pi\pi^*)$ | 3 |
|---------------------------|----|
| Root1[$T_1(3\pi\pi^*)$] | -752.667623 | -755.01570 | 53.1 |

| $T_1(3\pi\pi^*)$ Min |
|-----------------------|
| Root1[$T_1(3\pi\pi^*)$] | -752.669078 | -755.01813 | 51.6 |
Table S13. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol⁻¹) for complex 1 in the \(7(S_0/F)_0\), \(7(S_1(1\pi\pi^*)/F)_0\) and \(9(3\pi\pi^*/F)_0\) states along the relaxation pathway obtained by using 14 roots state-averaged CASPT2 calculations. The corresponding energy profiles are plotted in Figure 3 of the main article.

| Critical points | Complex 1 | RASSCF | CASPT2 |
|-----------------|-----------|--------|--------|
|                 |           | A.E.   | A.E.   | R.E.   |
| \(7(S_0/F)_0\)  | \(7(S_0/F)_0\) | \(-3398.152917\) | \(-3404.73065\) | 0.0 |
| Root1           | \(-3398.152138\) | \(-3404.72962\) | 0.6 |
| Root2           | \(-3398.148891\) | \(-3404.72560\) | 3.2 |
| Root3           | \(-3398.148235\) | \(-3404.72458\) | 3.8 |
| Root4           | \(-3398.146006\) | \(-3404.72607\) | 4.1 |
| Root5           | \(-3398.147147\) | \(-3404.72547\) | 4.5 |
| Root6           | \(-3398.146553\) | \(-3404.72274\) | 5.0 |
| Root7           | \(-3398.034092\) | \(-3404.62686\) | 65.1 |
| Root8           | \(-3398.033465\) | \(-3404.62686\) | |
| Root9           | \(-3398.030349\) | \(-3404.62686\) | |
| Root10          | \(-3398.029675\) | \(-3404.62686\) | |
| Root11          | \(-3398.029495\) | \(-3404.62686\) | |
| Root12          | \(-3398.026611\) | \(-3404.62686\) | |
| Root13          | \(-3398.027966\) | \(-3404.62686\) | |
| Root14          | \(-3398.027966\) | \(-3404.62686\) | |

Path \(7(S_1/F)_0\)\(\rightarrow\)1

| Critical points | Complex 1 | RASSCF | CASPT2 |
|-----------------|-----------|--------|--------|
|                 |           | A.E.   | A.E.   | R.E.   |
| Root1           | \(-3398.154954\) | \(-3404.73065\) | 0.0 |
| Root2           | \(-3398.154183\) | \(-3404.72962\) | 0.6 |
| Root3           | \(-3398.150936\) | \(-3404.72560\) | 3.2 |
| Root4           | \(-3398.150312\) | \(-3404.72458\) | 3.8 |
| Root5           | \(-3398.150052\) | \(-3404.72407\) | 4.1 |
| Root6           | \(-3398.148982\) | \(-3404.72274\) | 4.5 |
| Root7           | \(-3398.036276\) | \(-3404.62888\) | 63.9 |
| Root8           | \(-3398.035619\) | \(-3404.62888\) | |
| Root9           | \(-3398.031861\) | \(-3404.62888\) | |
| Root10          | \(-3398.031622\) | \(-3404.62888\) | |
| Root11          | \(-3398.030534\) | \(-3404.62888\) | |
| Root12          | \(-3398.029967\) | \(-3404.62888\) | |
| Root13          | \(-3398.028611\) | \(-3404.62888\) | |
| Root14          | \(-3398.027966\) | \(-3404.62888\) | |

Path \(7(S_1(1\pi\pi^*)/F)_0\)\(\rightarrow\)1

| Critical points | Complex 1 | RASSCF | CASPT2 |
|-----------------|-----------|--------|--------|
|                 |           | A.E.   | A.E.   | R.E.   |
| Root1           | \(-3398.128437\) | \(-3404.724216\) | 4.0 |
| Root2           | \(-3398.127715\) | \(-3404.724216\) | 4.0 |
| Root3           | \(-3398.124367\) | \(-3404.724216\) | 4.0 |
| Root4           | \(-3398.123783\) | \(-3404.724216\) | 4.0 |
| Root5           | \(-3398.123542\) | \(-3404.724216\) | 4.0 |
| Root6           | \(-3398.122457\) | \(-3404.724216\) | 4.0 |
| Root7           | \(-3398.121958\) | \(-3404.724216\) | 4.0 |
| Root8           | \(-3398.038749\) | \(-3404.62933\) | 63.6 (480 nm) |
| Root9           | \(-3398.038124\) | \(-3404.62933\) | 63.6 (480 nm) |
| 9(3ππ⁻/F)₀⁻¹³ |  |  |  |
|-----------------|--------|--------|--------|
| Root1           | -3398.033988 | -3404.63173 | 62.1 |
| Root2           | -3398.033325 | -3404.63086 | 62.6 |
| Root3           | -3398.030120 | -3404.62685 | 65.1 |
| Root4           | -3398.029522 | -3404.62576 | 65.8 |
| Root5           | -3398.029294 | -3404.62550 | 66.0 |
| Root6           | -3398.028161 | -3404.62448 | 66.6 |
| Root7           | -3398.027598 | -3404.62373 | 67.1 |
| Root8           | -3397.981101 |        |        |
| Root9           | -3397.980391 |        |        |
| Root10          | -3397.977038 |        |        |
| Root11          | -3397.976455 |        |        |
| Root12          | -3397.976235 |        |        |
| Root13          | -3397.975118 |        |        |
| Root14          | -3397.974619 |        |        |

| Path 9(3ππ⁻/F)₀⁻¹ |  |  |  |
|-------------------|--------|--------|--------|
| Root1             | -3398.039474 | -3404.63261 | 61.5 |
| Root2             | -3398.038795 |        |        |
| Root3             | -3398.035572 |        |        |
| Root4             | -3398.034960 |        |        |
| Root5             | -3398.034736 |        |        |
| Root6             | -3398.033603 |        |        |
| Root7             | -3398.033041 |        |        |
| Root8             | -3397.972992 |        |        |
| Root9             | -3397.972255 |        |        |
| Root10            | -3397.968911 |        |        |
| Root11            | -3397.968311 |        |        |
| Root12            | -3397.968086 |        |        |
| Root13            | -3397.967016 |        |        |
| Root14            | -3397.966528 |        |        |

| 9(3ππ⁺/F)₀ Min   |  |  |  |
|------------------|--------|--------|--------|
| Root1            | -3398.038773 | -3404.63350 | 61.0 |
| Root2            | -3398.038101 |        |        |
| Root3            | -3398.034899 |        |        |
| Root4            | -3398.034291 |        |        |
| Root5            | -3398.034064 |        |        |
| Root6            | -3398.032933 |        |        |
| Root7            | -3398.032373 |        |        |
| Root8            | -3397.972687 |        |        |
| Root9            | -3397.971960 |        |        |
| Root10           | -3397.968637 |        |        |
| Root11           | -3397.968040 |        |        |
| Root12           | -3397.967817 |        |        |
| Root13 | -3397.966746 |
|--------|--------------|
| Root14 | -3397.966261 |
Table S14. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol$^{-1}$) for complex 1 in the $^7$(S$_0^*/F$)$_0$ and $^5$(S$_0^*/D$)$_0$ states along the relaxation pathway obtained by using 7 or 5 roots state-averaged CASPT2 calculations. The corresponding energy profiles are plotted in Figure 3 of the main article.

| Critical points | Complex 1 | RASSCF | CASPT2 |
|----------------|-----------|--------|--------|
|                |           | A.E.   | A.E.   | R.E.   |
| $^7$(S$_0^*/F$)$_0$ − Min |           |        |        |        |
| Root1 $^7$(S$_0^*/F$)$_0$ | −3398.151722 | −3404.73042 | 0.0    |
| Root2          | −3398.150954 |        |        |        |
| Root3          | −3398.147719 |        |        |        |
| Root4          | −3398.147066 |        |        |        |
| Root5          | −3398.146843 |        |        |        |
| Root6          | −3398.145989 |        |        |        |
| Root7 $^7$(S$_0^*/F$)$_0$ | −3398.145401 |        |        |        |
| Path $^5$(S$_0^*/D$)$_0$−1 |           |        |        |        |
| Root1 $^5$(S$_0^*/D$)$_0$ | −3398.057670 | −3404.63514 | 59.8   |
| Root2          | −3398.057598 |        |        |        |
| Root3          | −3398.057338 |        |        |        |
| Root4          | −3398.056458 |        |        |        |
| Root5          | −3398.056291 |        |        |        |
| Path $^5$(S$_0^*/D$)$_0$−2 |           |        |        |        |
| Root1 $^5$(S$_0^*/D$)$_0$ | −3398.059538 | −3404.64025 | 56.6   |
| Root2          | −3398.059463 |        |        |        |
| Root3          | −3398.059202 |        |        |        |
| Root4          | −3398.058326 |        |        |        |
| Root5          | −3398.058143 |        |        |        |
| $^5$(S$_0^*/D$)$_0$−4 |           |        |        |        |
| Root1 $^5$(S$_0^*/D$)$_0$ | −3398.067729 | −3404.64687 | 52.4   |
| Root2          | −3398.067655 |        |        |        |
| Root3          | −3398.067395 |        |        |        |
| Root4          | −3398.066531 |        |        |        |
| Root5          | −3398.066345 |        |        |        |
| $^5$(S$_0^*/D$)$_0$ − Min |           |        |        |        |
| Root1 $^7$(S$_0^*/F$)$_0$ | −3398.173462 | −3404.72572 | 3.0    |
| Root2 $^7$(S$_0^*/F$)$_1$ | −3398.172768 | −3404.72484 | 3.5    |
| Root3 $^7$(S$_0^*/F$)$_2$ | −3398.169483 | −3404.72080 | 6.0    |
| Root4 $^7$(S$_0^*/F$)$_3$ | −3398.168870 | −3404.71969 | 6.7    |
| Root5 $^7$(S$_0^*/F$)$_4$ | −3398.168558 | −3404.71913 | 7.1    |
| Root6 $^7$(S$_0^*/F$)$_5$ | −3398.167533 | −3404.71841 | 7.5    |
| Root7 $^7$(S$_0^*/F$)$_6$ | −3398.166956 | −3404.71760 | 8.0    |
Table S15. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol⁻¹) for complex 2 along the relaxation pathway in the $^7(S_0/F_0)$ and $^9(3ππ*/F_0)$ states obtained by using 14 roots state–averaged CASPT2 calculations. The corresponding energy profiles are plotted in Figure 3 of the main article.

| Critical points | Complex 2 | RASSCF | CASPT2 |
|-----------------|-----------|--------|--------|
|                 |           | A.E.   | A.E.   | R.E.   |
| $^7(S_0/F_0)$−Min | |        |        |        |
| Root1 $^7(S_0/F_0)$ | -3435.870790 | -3442.86191 | 0.0 |
| Root2 $^7(S_0/F_4)$ | -3435.869498 |            |        |
| Root3 $^7(S_0/F_1)$ | -3435.866503 |            |        |
| Root4 $^7(S_0/F_2)$ | -3435.865781 |            |        |
| Root5 $^7(S_0/F_3)$ | -3435.865558 |            |        |
| Root6 $^7(S_0/F_5)$ | -3435.864786 |            |        |
| Root7 $^7(S_0/F_9)$ | -3435.864288 |            |        |
| Root8 $^7(S_1(1ππ*/F_0)$ | -3435.753031 | -3442.76348 | 61.8 (463 nm) |
| Root9 | -3435.751881 |        |        |
| Root10 | -3435.749028 |        |        |
| Root11 | -3435.748298 |        |        |
| Root12 | -3435.746088 |        |        |
| Root13 | -3435.747319 |        |        |
| Root14 | -3435.746762 |        |        |
| $^9(3ππ*/F_0)$−Min | |        |        |        |
| Root1 $^9(3ππ*/F_0)$ | -3435.758215 | -3442.76714 | 59.5 |
| Root2 | -3435.756961 |        |        |
| Root3 | -3435.754026 |        |        |
| Root4 | -3435.753344 |        |        |
| Root5 | -3435.753068 |        |        |
| Root6 | -3435.752128 |        |        |
| Root7 | -3435.751632 |        |        |
| Root8 | -3435.701840 |        |        |
| Root9 | -3435.700517 |        |        |
| Root10 | -3435.697471 |        |        |
| Root11 | -3435.696767 |        |        |
| Root12 | -3435.696570 |        |        |
| Root13 | -3435.695614 |        |        |
| Root14 | -3435.695192 |        |        |
Table S16. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol\(^{-1}\)) for complex 3 in the \(^7\langle S_0/F\rangle_0\), \(^7\langle S_1(1\pi\pi^*)/F\rangle_0\) and \(^9\langle 3\pi\pi^*/F\rangle_0\) states along the relaxation pathway obtained by using 14 roots state-averaged CASPT2 calculations. The corresponding energy profiles are plotted in Figure 3 of the main article.

| Critical points | Complex 3 | RASSCF | CASPT2 |
|----------------|-----------|--------|---------|
|                | \(^7\langle S_0/F\rangle_0\) \(-\) Min |        |         |
| Root1          | \(^7\langle S_0/F_0\rangle\)             | -3267.264125 | -3273.94838 | 0.0 |
| Root2          | \(^7\langle S_0/F_4\rangle\)             | -3267.263150 | -3273.94736 | 0.6 |
| Root3          | \(^7\langle S_0/F_1\rangle\)             | -3267.261949 | -3273.94546 | 1.8 |
| Root4          | \(^7\langle S_0/F_2\rangle\)             | -3267.260896 | -3273.94444 | 2.5 |
| Root5          | \(^7\langle S_0/F_3\rangle\)             | -3267.260313 | -3273.94349 | 3.1 |
| Root6          | \(^7\langle S_0/F_5\rangle\)             | -3267.260026 | -3273.94326 | 3.2 |
| Root7          | \(^7\langle S_0/F_6\rangle\)             | -3267.259969 | -3273.94303 | 3.4 |
| Root8          |                                           | -3267.142934 |            |     |
| Root9          | \(^7\langle S_1(1\pi\pi^*)/F\rangle_0\) | -3267.141990 | -3273.84819 | 62.9 (454nm) |
| Root10         |                                           | -3267.140855 |            |     |
| Root11         |                                           | -3267.139796 |            |     |
| Root12         |                                           | -3267.139142 |            |     |
| Root13         |                                           | -3267.138834 |            |     |
| Root14         |                                           | -3267.138679 |            |     |
|                | \(^7\langle S_1(1\pi\pi^*)/F\rangle_0\) \(-\) Min |        |         |
| Root1          |                                           | -3267.234669 |            |     |
| Root2          |                                           | -3267.233650 |            |     |
| Root3          |                                           | -3267.232556 |            |     |
| Root4          |                                           | -3267.231448 |            |     |
| Root5          |                                           | -3267.230846 |            |     |
| Root6          |                                           | -3267.230493 |            |     |
| Root7          |                                           | -3267.230416 |            |     |
| Root8          |                                           | -3267.144196 |            |     |
| Root9          | \(^7\langle S_1(1\pi\pi^*)/F_0\rangle\)  | -3267.143216 | -3273.85363 | 59.5 |
| Root10         |                                           | -3267.142128 |            |     |
| Root11         |                                           | -3267.141095 |            |     |
| Root12         |                                           | -3267.140522 |            |     |
| Root13         |                                           | -3267.139957 |            |     |
| Root14         |                                           | -3267.139647 |            |     |
|                | \(^9\langle 3\pi\pi^*/F\rangle_0\) \(-\) Min |        |         |
| Root1          | \(^9\langle 3\pi\pi^*/F_0\rangle\)      | -3267.138964 | -3273.85105 | 61.1 |
| Root2          | \(^9\langle 3\pi\pi^*/F_1\rangle\)      | -3267.137973 | -3273.84993 | 61.8 |
| Root3          | \(^9\langle 3\pi\pi^*/F_2\rangle\)      | -3267.136892 | -3273.84828 | 62.8 |
| Root4          | \(^9\langle 3\pi\pi^*/F_3\rangle\)      | -3267.135872 | -3273.84716 | 63.5 |
| Root5          | \(^9\langle 3\pi\pi^*/F_4\rangle\)      | -3267.135322 | -3273.84645 | 64.0 |
| Root6          | \(^9\langle 3\pi\pi^*/F_5\rangle\)      | -3267.134732 | -3273.84578 | 64.4 |
| Root7          | \(^9\langle 3\pi\pi^*/F_6\rangle\)      | -3267.134432 | -3273.84548 | 64.6 |
| Root8          |                                           | -3267.068724 |            |     |
| Root9          |                                           | -3267.067709 |            |     |
| Root  | Value       |
|-------|-------------|
| Root 10 | -3267.066618 |
| Root 11 | -3267.065510 |
| Root 12 | -3267.064900 |
| Root 13 | -3267.064553 |
| Root 14 | -3267.064495 |

| $\frac{(\beta \pi \pi^* / F)_{0-13} - \text{Min}}{\beta \pi \pi^*/F}$ | Value       |
|---------------------------------|-------------|
| Root 1 $\frac{(\beta \pi \pi^* / F)_{0}}{\beta \pi \pi^*/F}$ | -3267.147006 | -3273.85792 | 56.8 |
| Root 2 | -3267.145978 |
| Root 3 | -3267.145044 |
| Root 4 | -3267.144003 |
| Root 5 | -3267.143247 |
| Root 6 | -3267.143095 |
| Root 7 | -3267.142854 |
| Root 8 | -3267.089798 |
| Root 9 | -3267.088708 |
| Root 10 | -3267.087652 |
| Root 11 | -3267.086628 |
| Root 12 | -3267.085992 |
| Root 13 | -3267.085752 |
| Root 14 | -3267.085679 |
Table S17. Absolute energies (A.E., Hartree) and relative energies (R.E., kcal mol\(^{-1}\)) for the optimized structures of complex 4 along the relaxation pathway in the \(^7(S_0/F)\) and \(^9(3\pi\pi^*/F)\) states obtained by using 14 roots state-averaged CASPT2 calculations. The corresponding energy profiles are plotted in Figure 3 of the main article.

| Critical points | Complex 4 | RASSCF | CASPT2 |
|-----------------|-----------|--------|--------|
|                 |           | A.E.   | A.E.   | R.E.   |
| \(^7(S_0/F)\) 0−Min |           |        |        |        |
| Root1 \(^7(S_0/F_0)\) | -3583.513484 | -3590.61563 | 0.0    |
| Root2 \(^7(S_0/F_4)\) | -3583.512612 |        |        |        |
| Root3 \(^7(S_0/F_1)\) | -3583.511040 |        |        |        |
| Root4 \(^7(S_0/F_2)\) | -3583.510771 |        |        |        |
| Root5 \(^7(S_0/F_3)\) | -3583.510463 |        |        |        |
| Root6 \(^7(S_0/F_5)\) | -3583.510447 |        |        |        |
| Root7 \(^7(S_0/F_0)\) | -3583.509895 |        |        |        |
| Root8 \(^7(S_1(1\pi\pi^*)/F)\) | -3583.393478 | -3590.51635 | 62.3 (459 nm) |
| Root9 | -3583.392587 |        |        |        |
| Root10 | -3583.390999 |        |        |        |
| Root11 | -3583.390727 |        |        |        |
| Root12 | -3583.390506 |        |        |        |
| Root13 | -3583.390407 |        |        |        |
| Root14 | -3583.389896 |        |        |        |
| \(^9(3\pi\pi^*/F)\) 0−Min |           |        |        |        |
| Root1 \(^9(3\pi\pi^*/F_0)\) | -3583.394500 | -3590.52722 | 55.5 |
| Root2 | -3583.393558 |        |        |        |
| Root3 | -3583.391930 |        |        |        |
| Root4 | -3583.391614 |        |        |        |
| Root5 | -3583.391394 |        |        |        |
| Root6 | -3583.391055 |        |        |        |
| Root7 | -3583.390553 |        |        |        |
| Root8 | -3583.326571 |        |        |        |
| Root9 | -3583.325658 |        |        |        |
| Root10 | -3583.324075 |        |        |        |
| Root11 | -3583.323744 |        |        |        |
| Root12 | -3583.323465 |        |        |        |
| Root13 | -3583.323201 |        |        |        |
| Root14 | -3583.322720 |        |        |        |
3.9 Cartesian Coordinates

a) antenna PPPD

\( S_0 \) - Min

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| N       | 3.619019594 | -1.993887644 | 0.041572265 |
| O       | 1.504822465  | 2.236726756  | -0.244204849 |
| O       | -1.499185457 | 2.259251879  | -0.19629320  |
| H       | 1.610135278  | -1.791768839 | -0.151467536 |
| H       | 3.783141055  | 1.842924387  | 0.12367590   |
| H       | 5.660961925  | -1.994679042 | 0.227780584  |
| H       | 5.870127292  | 0.467054084  | 0.28993873   |
| H       | -0.013312687 | -0.650519483 | 0.154905892  |
| H       | -1.620597737 | -1.691510816 | -0.68486714  |
| H       | -3.679574357 | 1.821221731  | 0.561096803  |
| H       | -3.698733263 | -2.971772550 | -0.54072459  |
| H       | -5.779693488 | 0.539627865  | 0.72651170   |
| H       | -5.800662882 | -1.872780229 | 0.17354975   |
| C       | 1.268929239  | 1.041749101  | -0.10925965  |
| C       | 2.514526185  | 0.15206963   | 0.007934595  |
| C       | 2.525312352  | 1.243855334  | -0.039883041 |
| C       | 3.748243038  | 0.771104551  | 0.107600203  |
| C       | 4.789281507  | -1.365089894 | 0.16125944   |
| C       | 4.903238933  | 0.004057472  | 0.196431489  |
| C       | -0.01185897  | 0.401418885  | -0.037043879 |
| C       | -1.246336080 | 1.060844621  | -0.10321698  |
| C       | -2.491343056 | 0.167271912  | -0.031259315 |
| C       | -2.516306321 | -1.192782538 | -0.350730034 |
| C       | -3.697662880 | 0.770734434  | 0.344479985  |
| C       | -3.702501872 | -1.926497424 | -0.280762165 |
| C       | -4.864943933 | 0.049277747  | 0.42689135   |
| C       | -4.884070826 | -1.310092122 | 0.116017699  |

\( S_1 (\pi \pi^+)^- \) - Min

| Element | X         | Y         | Z         |
|---------|-----------|-----------|-----------|
| N       | 3.514335253 | -2.002461147 | 0.063081003 |
| O       | 1.424628103 | 2.300000167  | -0.237001016 |
| O       | -1.455375106 | 2.283792167  | -0.1991220016 |
| H       | 1.539680111  | -1.744473125 | -0.112082006 |
| H       | 3.922877282  | 1.850801133  | 0.089101008  |
| H       | 5.576259401  | -2.087200152  | 0.237265015  |
| H       | 5.886474424  | 0.408084032  | 0.26002120  |
| H       | 0.019412000  | -0.625234043  | 0.167632012  |
| H       | -1.594215113 | -1.659471820 | -0.689989050 |
| H       | -3.73483268  | 1.814352129  | 0.570658041  |
| H       | -3.635295261 | -2.970222216 | -0.546623038 |
| H       | -5.799236416 | 0.471557033  | 0.727956052  |
| H       | -5.756357417 | -1.926964138 | 0.168907012  |
| C       | 1.358941098  | 1.091430076  | -0.11091009  |
| C       | 2.514593178  | 0.221986014  | -0.02912002  |
| C       | 2.466794180  | -1.213570086  | -0.017794003 |
| C       | 3.813619273  | 0.788196055  | 0.088102006  |
| C       | 4.730743241  | -1.422612102  | 0.167774012  |
| C       | 4.904319354  | -0.017678002  | 0.180134015  |
| C       | 0.018294001  | 0.440075029  | -0.217681003  |
| C       | -1.285528095 | 1.088138081  | -0.107854007 |
| C       | -2.500661680 | 0.165974015  | -0.033080002  |
| C       | -2.493247179 | -1.17653082  | -0.35498023  |
| C       | -3.720198268 | 0.765970548  | 0.346516026  |
|   |   |   |   |   |
|---|---|---|---|---|
| C | -3.661324262 | -1.932475138 | -0.285689022 |
| C | -4.875074352 | 0.008147001 | 0.425684033 |
| C | -4.854035350 | -1.342039097 | 0.111883009 |

\[ T_1 (^{13}\text{C}-\text{N})-\text{Min} \]

|   |   |   |   |   |
|---|---|---|---|---|
| N | 3.783596274 | -1.767410127 | 0.044313001 |
| O | 1.305066092 | 2.343248168 | -0.123877007 |
| O | -1.569836113 | 2.166771545 | -0.144050011 |
| H | 0.016459000 | -0.670929049 | 0.017056002 |
| H | 1.768451125 | -1.740255127 | -0.043463005 |
| H | 3.710350269 | 2.071470418 | 0.001494000 |
| H | 5.838398422 | -1.631691117 | 0.123605010 |
| H | 5.851897422 | 0.846762060 | 0.096988008 |
| H | -1.525728109 | -1.892595134 | -0.229050017 |
| H | -3.557702547 | -3.227682300 | -0.124964011 |
| H | -3.820772737 | 1.680513122 | 0.121802008 |
| H | -5.766602415 | -2.130798155 | 0.105750007 |
| H | -5.884761424 | 0.342701023 | 0.227310007 |
| C | 1.251032088 | -0.919803107 | -0.075216005 |
| C | 2.501536180 | 0.304440021 | -0.021066001 |
| C | 2.639419191 | -1.110060079 | -0.006485006 |
| C | 3.723594268 | 0.999674070 | 0.014769004 |
| C | 4.918027352 | 0.308999021 | 0.067272007 |
| C | 4.921754353 | -1.068340777 | 0.082763004 |
| C | -0.125920000 | 0.396283030 | -0.056880006 |
| C | -1.325077093 | 0.964965070 | -0.105075006 |
| C | -2.461678179 | -1.379689101 | -0.120741008 |
| C | -2.513787183 | 0.022690011 | -0.048910006 |
| C | -3.624163260 | -2.149331517 | -0.065299007 |
| C | -3.783596274 | 0.999674070 | 0.014769004 |
| C | 4.918027352 | 0.308999021 | 0.067272007 |

\[ \text{Cl}(\text{S}_1/\text{S}_0) \]

|   |   |   |   |   |
|---|---|---|---|---|
| N | 4.328666309 | 1.622549115 | 0.592687044 |
| O | 1.057947074 | -1.437494106 | -0.685608050 |
| O | -0.895157065 | -0.145548012 | 1.823549129 |
| H | 2.402025171 | 2.160202153 | 0.711078049 |
| C | 3.178737228 | -1.765416129 | -0.675284051 |
| C | 5.996634010 | -1.276076090 | -0.426458029 |
| C | 6.250178450 | 0.960575068 | 0.420315032 |
| C | -0.292122018 | 0.802974060 | -1.344250999 |
| C | -2.588574185 | 2.183549157 | -0.799140060 |
| C | -2.931445211 | -1.616608116 | 1.146326083 |
| C | -4.937498355 | 2.029681414 | -1.480507109 |
| C | -5.263785380 | -1.778466127 | 0.431315029 |
| H | -6.300826252 | 0.046681003 | -0.05562061 |
| C | 1.230137091 | -0.286360200 | -0.231001014 |
| C | 2.542286183 | 0.144274012 | -0.017265000 |
| C | 3.051048218 | 1.349361010 | 0.444459030 |
| C | 3.529674255 | -0.827685061 | -0.321572023 |
| C | 4.853653348 | -0.546924039 | -0.179227011 |
| C | 5.226389376 | 0.697007052 | 0.286873019 |
| C | -0.186260002 | 0.519575037 | -0.295825021 |
| C | -1.124060708 | 0.257740101 | 0.671815050 |
| C | -2.571422185 | 0.296547020 | 0.252167019 |
| C | -3.150852227 | 1.312786094 | -0.508808037 |
| C | -3.363727243 | -0.806920056 | 0.583861039 |
|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| C   | -4.497702324 | 1.227312089 | -0.906723065 |     |     |
| C   | -4.687172338 | -0.900238066 | 0.179021013  |     |     |
| C   | -5.269380381 | 0.119984009  | -0.566866041 |     |     |

**STC(S1/T1)**

|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| N   | 4.336544314 | 1.636199120 | 0.596264044 |     |     |
| O   | 1.018344073 | -1.463440105 | -0.694250049 |     |     |
| C   | -0.877543062 | -0.137983010 | 1.817007133  |     |     |
| H   | 2.378379171 | 2.158334158  | 0.709171053  |     |     |
| H   | 3.191593229 | -1.775158129 | -0.677196047 |     |     |
| H   | 5.622531406 | -1.275324092 | -0.566866041 |     |     |
| H   | -0.348116025 | 0.885916064  | -1.266237092 |     |     |
| H   | -2.571150188 | 2.173001568  | -0.795785055 |     |     |
| H   | -2.925502212 | -1.602411115 | 1.158834081  |     |     |
| H   | -4.924815352 | 2.033249145  | -1.480227105 |     |     |
| H   | -5.258578376 | -1.768588129 | 0.445755033  |     |     |
| H   | -6.288977451 | 0.054620003  | -0.881394063 |     |     |
| C   | 1.210648085  | -0.290555019 | 0.531479038  |     |     |
| C   | 2.553855183  | 0.133761012  | -0.020769000 |     |     |
| C   | 3.049197220  | 1.363124096  | 0.445920303  |     |     |
| C   | 3.538947255  | -0.829373062 | -0.322479023 |     |     |
| C   | 4.868802348  | -0.545010400 | -0.175464010 |     |     |
| C   | 5.228785374  | 0.711562051  | 0.292356021  |     |     |
| C   | -0.023558003 | 0.531479038  | -0.278323018 |     |     |
| C   | -1.112783082 | 0.249075016  | 0.579755048  |     |     |
| C   | -2.564512183 | -0.288894021 | 0.240349015  |     |     |
| C   | -3.149308226 | 1.311338096  | -0.511138036 |     |     |
| C   | -3.363201241 | -0.806341056 | 0.584908043  |     |     |
| C   | -4.490778325 | 1.232842086  | -0.904850686 |     |     |
| C   | -4.680031334 | -0.89896062  | 0.182529013  |     |     |
| C   | -5.260437381 | 0.124101008  | -0.665982040 |     |     |

**Complex 1**

S0/F0 - Min

|     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|
| N   | 10.103333407 | 25.292269148 | -1.408298153 |     |     |
| C   | 6.319031358  | 24.552722077 | 6.488052932  |     |     |
| C   | 6.377221609  | 23.150770781 | 6.451621851  |     |     |
| C   | 6.763047011  | 25.275791950 | 5.418998851  |     |     |
| C   | 6.883983587  | 22.50357861  | 5.356216034  |     |     |
| C   | 7.289075545  | 24.619299862 | 4.289904658  |     |     |
| C   | 7.359172480  | 23.235285928 | 4.243074567  |     |     |
| C   | 7.90120718   | 22.445187350 | 3.069957023  |     |     |
| C   | 8.41586375   | 23.115107684 | 1.957075413  |     |     |
| C   | 8.975769298  | 22.437534582 | 0.850616608  |     |     |
| C   | 9.534368553  | 23.23165006  | -0.31096883  |     |     |
| C   | 9.610651459  | 24.602171559 | -0.36550347  |     |     |
| C   | 10.01120633  | 22.521906905 | -1.42625047  |     |     |
| C   | 10.513477271 | 23.207271851 | -2.50024940  |     |     |
| C   | 10.536096556 | 24.602182814 | -2.443790379 |     |     |
| O   | 7.826459693  | 21.210129718 | 3.184425555  |     |     |
| O   | 9.062124135  | 21.211580193 | 0.727682827  |     |     |
| H   | 5.919972794  | 25.051606069 | 7.35352708  |     |     |
| H   | 6.021143488  | 22.58168348  | 7.29213846  |     |     |
| H   | 6.722440426  | 26.35037080  | 5.43190082  |     |     |
| H   | 6.914587940  | 21.438932292 | 5.310608761 |     |     |
| H   | 7.625523905  | 25.216064645 | 3.465225048 |     |     |
S_{i}/F_{0}-Min

N 10.086076021 25.321637740 -1.454680010
C 6.317484367 24.656037670 6.512563903
C 6.345973455 23.248303688 6.503011423
C 6.801202649 25.342852022 5.408522930
C 6.838456643 22.55908785 5.433838547
C 7.307902105 24.678240127 4.30978313
C 7.34308048 23.251723073 4.280281426
C 7.837518788 22.46219974 3.19338669
C 8.434143641 23.17405921 1.943049935
C 8.97086696 22.489036086 0.807488143
C 9.535974818 23.26398143 -0.353547490
C 9.604629613 24.653975122 -0.423742423
C 10.020188056 22.549759445 -1.458552100
C 10.521190151 23.24571206 -2.539203545
C 10.529936028 24.630926202 -2.489700792
O 7.806867641 21.259650681 3.196617592
O 9.084153361 21.27052696 0.706299944
H 5.928952593 25.18888321 7.361361231
H 5.975483821 22.706318196 7.357019210
H 6.783086855 26.419920497 5.404586549
H 6.848017077 21.483275584 5.431849719
H 7.662786157 25.261672083 3.481825889
H 8.435582987 24.239881272 1.922584995
H 9.262910864 25.268237870 0.387801202
H 10.01082563 21.473662571 -1.445754155
H 10.897163588 22.732680928 -3.405075439
H 10.912161035 25.205625418 -3.314410030
N 2.307585188 21.07897165 -0.924932467
N 6.513460636 18.595894988 3.560730805
N 10.375071131 18.594666323 0.346781080
N 14.562586246 21.064726363 4.885380312
C 2.435500077 22.30937917 -0.375397393
C 3.305145671 20.208901233 -0.650749388
C 3.506452041 22.700831983 0.41620092
| C | 4.265192244 | 17.721876935 | 4.986475334 |
| C | 4.375036423 | 19.044178784 | 4.585140286 |
| C | 4.417011530 | 20.504237193 | 0.138737405 |
| C | 4.511906822 | 21.78620852 | 0.674283736 |
| C | 4.731236647 | 13.81362071 | 0.08448109 |
| C | 4.925056943 | 15.19223995 | 0.351460690 |
| C | 5.281120353 | 16.83682176 | 4.658914918 |
| C | 5.340443573 | 18.12993331 | 0.200391301 |
| C | 5.517471434 | 19.49782753 | 0.41847704 |
| C | 5.49870002 | 19.44036399 | 3.876477074 |
| C | 5.770764728 | 13.04459725 | -0.414440017 |
| C | 5.61482177 | 17.75319771 | 0.12289796 |
| C | 5.37350628 | 17.30643855 | 3.951131103 |
| C | 5.396168409 | 17.23574858 | 0.41866804 |
| C | 7.007937638 | 13.62274680 | -0.646595165 |
| C | 7.20391860 | 14.97071483 | -0.373534075 |
| C | 9.660070404 | 14.96153805 | 4.284762055 |
| C | 9.861678499 | 13.61577121 | 4.59379758 |
| C | 10.47627920 | 17.22785021 | 3.501461112 |
| C | 10.52268456 | 17.30191058 | -0.042600611 |
| C | 10.706040549 | 15.74739108 | 3.79565068 |
| C | 11.099102604 | 13.03531713 | 4.31540921 |
| C | 11.39106652 | 19.43525177 | 0.022013943 |
| C | 11.36545575 | 19.49197701 | 3.48631541 |
| C | 11.53207052 | 18.12311156 | 3.727631002 |
| C | 11.59157278 | 16.83185314 | -0.76182968 |
| C | 11.94614894 | 15.15493064 | 3.56486161 |
| C | 12.139658183 | 13.80699529 | 3.81961629 |
| C | 12.378169815 | 21.77894687 | 3.26270681 |
| C | 12.465219837 | 20.49470925 | 3.79576315 |
| C | 12.50534115 | 19.03632213 | -0.69801493 |
| C | 12.606305816 | 17.71267405 | -1.10048152 |
| C | 13.379391677 | 22.69283079 | 3.536298067 |
| C | 13.567326541 | 20.19657973 | 4.59754480 |
| C | 14.441319866 | 22.29821822 | 4.339440014 |
| O | 6.611200108 | 19.97914337 | 0.92178999 |
| O | 7.568103951 | 17.57172684 | 0.83979535 |
| O | 9.306908619 | 17.56689471 | 3.073260063 |
| O | 10.28764316 | 19.97462078 | 2.967818554 |
| H | 1.632143882 | 23.01020747 | -0.59061312 |
| H | 3.193886666 | 19.22757098 | -1.10277674 |
| H | 3.396950716 | 17.38432012 | 5.54172920 |
| H | 3.547641796 | 23.70298240 | 0.62129977 |
| H | 3.603204571 | 19.76711633 | 4.81164252 |
| H | 3.765181023 | 13.36218314 | 0.276111306 |
| H | 4.10891323 | 15.74732960 | 0.749777073 |
| H | 4.413890903 | 17.76250508 | -0.190830148 |
| H | 5.230939983 | 15.70524701 | 4.94467762 |
| H | 5.367655793 | 22.04974540 | 1.28539452 |
| H | 5.615469525 | 20.46328565 | 3.536404056 |
| H | 5.616557524 | 11.99342479 | -0.62493427 |
| H | 7.188691399 | 16.64860009 | 3.667744775 |
| H | 7.821931523 | 13.03152536 | -1.040912218 |
| H | 8.167440276 | 15.42300090 | -0.560669942 |
| H | 8.702095552 | 15.41313165 | 4.473161554 |
| H | 9.046941929 | 13.01896198 | 4.93841397 |
| H | 9.691732786 | 16.64916360 | 0.249724496 |
| H | 11.252856223 | 11.98277647 | 4.518550817 |
| H | 11.285198107 | 20.455951547 | 0.371021515 |
|      | Coordinates                  | Value   |
|------|------------------------------|---------|
|      | X                            | Y       | Z       |
| H    | 11.528263844                 | 22.043292854 | 2.644536907 |
| H    | 11.636523011                 | 15.789515480 | -1.046977150 |
| H    | 12.450595632                 | 17.754213178 | 4.135977839 |
| H    | 12.762926639                 | 15.745320865 | 3.607995353 |
| H    | 13.279772767                 | 19.754761974 | -0.929925471 |
| H    | 13.343270211                 | 23.696571239 | 3.136813652 |
| H    | 13.488100192                 | 17.372038050 | -1.663870603 |
| H    | 13.667126608                 | 19.214124623 | 5.048744685 |
| H    | 15.241764835                 | 22.997827290 | 4.567642781 |
| Eu   | 8.439468937                  | 19.299507738 | 1.958111346 |
| T_{1f}/F_{0-Min} |                        |         |
| N    | 10.021095717                 | 25.372231519 | -1.408371196 |
| C    | 6.357284454                  | 24.585620328 | 6.531679309 |
| C    | 6.390771097                  | 23.179028534 | 6.479718014 |
| C    | 6.820633170                  | 25.31247723 | 5.457993652 |
| C    | 6.882202117                  | 22.537580740 | 5.372252511 |
| C    | 7.326994630                  | 24.648541826 | 4.325750411 |
| C    | 7.368537129                  | 23.277826968 | 4.267726596 |
| C    | 7.904960370                  | 22.490979754 | 3.080921581 |
| C    | 8.46719838                   | 23.12300332 | 1.935630823 |
| C    | 9.004472391                  | 22.458132606 | 0.819002718 |
| C    | 9.528027449                  | 23.270707640 | -0.346198680 |
| C    | 9.549263025                  | 24.650256572 | -0.381357458 |
| C    | 10.042212440                 | 22.602287648 | -1.477951807 |
| C    | 10.52790129                  | 23.330990480 | -2.528534226 |
| C    | 10.486687737                 | 24.72944752 | -2.440165790 |
| O    | 7.789916231                  | 21.277907507 | 3.221008361 |
| O    | 9.103645578                  | 21.240025645 | 0.682870807 |
| C    | 5.971230331                  | 25.084561506 | 7.402863761 |
| C    | 6.028023586                  | 22.608079795 | 7.316607383 |
| C    | 6.800414334                  | 26.387756099 | 5.478060625 |
| C    | 6.892240366                  | 21.465144129 | 5.332873597 |
| H    | 7.680607590                  | 25.239800494 | 3.503289144 |
| C    | 8.474181117                  | 24.191637828 | 1.938577541 |
| C    | 9.180082226                  | 25.230325566 | 0.439532247 |
| H    | 10.057018830                 | 21.530364183 | -1.48558466 |
| H    | 10.919026173                 | 22.85850177 | -3.40695277 |
| H    | 10.85798721                  | 25.33027193 | -3.25308786 |
| C    | 2.330581553                  | 21.060878704 | -1.00802277 |
| N    | 6.505493939                  | 18.11647373 | 3.582562388 |
| C    | 10.385956248                 | 18.577307288 | 0.352026068 |
| N    | 14.540852915                 | 21.070064629 | 4.916856929 |
| C    | 2.450435168                  | 22.290872025 | -0.469332530 |
| C    | 3.323499078                  | 20.194735804 | -0.708933405 |
| C    | 3.508541916                  | 22.696821464 | 0.334889883 |
| C    | 4.260497018                  | 17.736271651 | 5.016622985 |
| C    | 4.368708522                  | 19.057797664 | 4.611978442 |
| C    | 4.422283395                  | 20.497665283 | 0.095916811 |
| C    | 4.509553497                  | 21.784873055 | 0.619440214 |
| C    | 4.723018366                  | 13.810497118 | 0.126664941 |
| C    | 4.922150543                  | 15.157830534 | 0.37913379 |
| C    | 5.275091998                  | 16.853198465 | 4.684761269 |
| C    | 5.345994383                  | 18.125988925 | 0.181565471 |
| C    | 5.516723140                  | 19.494439709 | 0.421019219 |
| C    | 5.489477053                  | 19.455622483 | 3.897619657 |
| C    | 5.755273519                  | 13.037456604 | -0.384174142 |
| C    | 6.159874987                  | 15.748294107 | 0.131323256 |
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 6.369358522 | 17.321199469 | 3.973571854 |
| C    | 6.395229363 | 17.228717167 | 0.421881889 |
| C    | 6.972503957 | 13.624732737 | 4.579334196 |
| C    | 10.477635398 | 17.27402754  | 3.497352632 |
| C    | 10.593308080 | 17.289521437 | -0.047391744 |
| C    | 10.70607129  | 15.747786319 | 3.794614073 |
| C    | 11.051765098 | 17.228717167 | 0.421881889 |
| C    | 11.354398754 | 19.492252063 | 3.503737309 |
| C    | 11.533211778 | 18.123200865 | 3.724541924 |
| O    | 6.591024966 | 19.972222729 | 0.950211714 |
| O    | 7.562385302 | 17.56396125  | 3.012968274 |
| H    | 1.651082828 | 22.996288342 | -0.705364660 |
| O    | 8.714784551 | 15.423824992 | 4.502779589 |
| H    | 9.062522235 | 13.032341302 | 4.985268871 |
| H    | 9.708176747 | 16.626143716 | 0.245915452 |
| Eu   | 8.445893947 | 19.306111061 | 1.952377637 |
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| C       | 11.531708460 | 18.121342331 | 3.726507156 |
| C       | 11.583911764 | 16.825310495 | 3.726507156 |
| C       | 11.946538771 | 15.150206804 | 3.570944820 |
| C       | 12.140409688 | 13.801986036 | 3.832939386 |
| C       | 12.371650870 | 21.774720017 | 3.247422080 |
| C       | 12.461404506 | 20.493386451 | 3.785469128 |
| O       | 6.614383945 | 19.973622678 | 0.920643131 |
| O       | 7.567026895 | 17.76623109  | 0.840913317 |
| O       | 8.162154202 | 15.412873490 | 0.290290859 |
| H       | 1.637800109 | 23.006970912 | -0.595736126 |
| H       | 3.197643609 | 19.220413266 | -1.098051574 |
| H       | 3.557735275 | 23.703933395 | 0.808373535 |
| H       | 3.608964485 | 19.767340478 | 4.807906686 |
| H       | 3.760253308 | 13.356132747 | 0.290290859 |
| H       | 4.107763806 | 15.744911226 | 0.757503981 |
| H       | 4.414798828 | 17.760245482 | -1.095634455 |
| H       | 5.23909730 | 15.795637336 | 4.948859876 |
| H       | 5.379531250 | 22.047135231 | 1.273571910 |
| H       | 5.627654324 | 20.460409585 | 3.525356119 |
| H       | 5.607740653 | 11.986088820 | -0.611363646 |
| H       | 7.191717562 | 16.649470183 | 3.665985821 |
| H       | 7.813179408 | 13.020766206 | -1.036050444 |
| H       | 8.162771949 | 15.412883490 | -0.561325248 |
| H       | 8.702884280 | 15.412754106 | 4.479262349 |
| H       | 9.04864705 | 13.021166343 | 4.956707647 |
| H       | 9.685514064 | 16.643574084 | 0.252553462 |
| H       | 11.254727642 | 11.983719569 | 4.543461032 |
| H       | 11.26954025 | 20.450165285 | 0.369128564 |
| H       | 11.516826774 | 22.03829984 | 2.634736062 |
| H       | 11.629204040 | 15.78311965 | -1.042094072 |
| H       | 12.452344008 | 17.755458401 | -4.312749143 |
| H       | 12.762872430 | 15.739207864 | 3.174209895 |
| H       | 13.106708867 | 13.352385351 | 3.646013010 |
| H       | 13.266796732 | 19.751020002 | -0.932182153 |
| H       | 13.338220299 | 23.690970585 | 3.108063780 |
| H       | 13.459142264 | 17.367322680 | -1.663808955 |
| H       | 13.666795956 | 19.217658793 | 5.040334693 |
| H       | 15.242801535 | 22.997111027 | 4.533660680 |
| Eu      | 8.440641551 | 19.295623948 | 1.954667651 |

b) antenna para-Br-PPPD

So-Mn

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| N       | 4.850033733 | -2.316309775 | -0.368846137 |
| O       | 0.503563043 | 2.684911644 | -0.147025099 |
| O       | 3.404581298 | 2.175713329 | -0.062655562 |
| H       | -0.342433461 | -1.260553231 | 0.060778362 |
| H       | -1.783707009 | 2.731937975 | -0.157262546 |
| H       | -2.632762983 | -2.102965642 | 0.124183025 |
| H       | -4.107651923 | 1.902769011 | -0.093992458 |
| H       | 1.448793093 | -0.443916708 | -0.007935394 |
| H       | 2.931717071 | -1.751786407 | -0.743230965 |
S\(_1^{(\pi\pi^*)}\)-Min

N  
-5.195116376  
-1.998251145  
1.144502083

O  
-0.661522050  
2.41909174  
1.23454088

O  
-2.781181199  
1.468430104  
-1.033259077

H  
0.225639015  
-0.962449070  
-0.726084050

H  
1.902694138  
2.560581184  
1.100734081

H  
2.432099176  
-1.602483116  
-1.490371105

H  
4.126267299  
1.881007136  
0.371623026

H  
-1.518957107  
-0.473230032  
1.32150093

H  
-3.27086234  
-1.539791111  
1.61051118

H  
-5.047382365  
0.823565061  
-1.470889106

H  
-7.127218513  
-2.314294166  
0.551938041

H  
-7.126658511  
-0.509241036  
-1.153071082

C  
0.860183063  
0.887117064  
0.268678022

C  
1.050119077  
-0.332196024  
-0.47860033

C  
2.028017148  
1.651213117  
0.546331038

C  
3.204813167  
-0.701560051  
-0.921872065

C  
3.268031237  
1.284613095  
0.141845009

C  
3.419378248  
0.088598009  
-0.619042045

C  
-0.401349029  
1.35384095  
0.687627052

C  
-1.561271112  
0.366640028  
0.624010045

C  
-2.740474196  
0.601638045  
-0.187027015

C  
-4.088224296  
-1.269223091  
0.968926067

C  
-3.972227283  
-0.239972019  
0.036704004

C  
-5.100616369  
0.034904002  
-0.74565052

C  
-6.246581447  
-1.713065126  
0.390747026

C  
-6.243950452  
-0.69333050  
-0.568168039

Br  
5.157937372  
-0.458535034  
-1.177576084

T\(_1^{(\pi\pi^*)}\)-Min

N  
-4.818948348  
-2.385788171  
0.153827011

O  
-0.603272044  
2.709042195  
0.108701008

O  
-3.415753246  
2.136926155  
0.051873002

H  
0.39786024  
-1.258364093  
-0.007781001

H  
1.842454134  
2.805210201  
0.058470006

H  
2.631739189  
-2.063094149  
-0.108253007

H  
4.12006295  
1.959307139  
-0.045577005

H  
-1.447609107  
-0.457846034  
0.062257005

H  
-2.86878205  
1.857132135  
0.328897022
| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| H       | -5.619540406 | 1.360173097 | -0.210571013 |
| H       | -6.822888492 | -2.735080197 | -0.033895004 |
| H       | -7.435795536 | -0.341450027 | -0.278602021 |
| C       | 0.871260061 | 0.883008066 | 0.037137003 |
| C       | 1.157585085 | -0.527215039 | -0.014030002 |
| C       | 2.016184147 | 1.747470125 | 0.021641000 |
| C       | 2.453000175 | -1.002892071 | -0.072231006 |
| C       | 3.294455237 | 1.272163094 | -0.036440000 |
| C       | 3.532120255 | -1.084040047 | -0.084077004 |
| C       | -0.419498030 | 1.486596108 | 0.096778004 |
| C       | 1.623612115 | 0.594348041 | 0.087460008 |
| C       | 3.022637215 | 1.000465073 | 0.089688008 |
| C       | 3.857042806 | -1.462643106 | 0.18395012 |
| C       | -0.804082959 | -0.092472004 | 0.052976003 |
| C       | -6.064844437 | -0.191395140 | -0.011515003 |
| Br      | 5.326313381 | -0.771343057 | -0.165837011 |

**Cl(S/0)**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| N       | -5.833729417 | -1.477652108 | 1.408388103 |
| O       | -0.841800060 | 1.504042108 | 0.904224068 |
| O       | -2.441710178 | -0.367270024 | -1.684636121 |
| H       | 1.229139089 | -1.485928106 | -0.934939066 |
| H       | 1.151068082 | 2.258774164 | 1.085520077 |
| H       | 3.483684251 | -1.026476072 | -1.598860114 |
| H       | 3.520944255 | 2.547689183 | 0.659278047 |
| H       | -1.616377114 | -0.948293070 | 1.572484116 |
| H       | -3.935355282 | -2.143374153 | 1.628096115 |
| H       | -4.642258334 | 0.650351044 | -1.550159112 |
| H       | -7.697654553 | -0.677113051 | 1.12572609 |
| H       | -6.977094505 | 0.774024054 | -0.765716056 |
| C       | 0.933056068 | 0.411380028 | 0.068331007 |
| C       | 1.483071119 | -0.587290045 | -0.614240042 |
| C       | 1.483071119 | 1.547261110 | 0.512195036 |
| C       | 2.49447213 | -0.327683026 | -0.991520073 |
| C       | 2.994211261 | 1.709142124 | 0.289199023 |
| C       | 3.610270262 | 0.827888059 | -0.598523043 |
| C       | -0.373519026 | 0.453436035 | 0.455969032 |
| C       | -1.437630104 | -0.647407046 | 0.486412033 |
| C       | -2.581845188 | -0.668080048 | -0.510249039 |
| C       | -4.512653273 | -1.504899111 | 1.010265071 |
| C       | -4.36844292 | -0.893540595 | -0.073450003 |
| C       | -4.960711355 | 0.032602002 | -0.72912053 |
| C       | -6.676555483 | -0.694701051 | 0.763170503 |
| C       | -6.270859453 | 0.110994007 | -0.290450019 |
| Br      | 5.374983385 | 1.140934084 | -1.203391086 |

**STC(S/1)**

| Element | X       | Y       | Z       |
|---------|---------|---------|---------|
| N       | -5.195116376 | -1.998251145 | 1.144502083 |
| O       | -0.661522050 | 2.413909174 | 1.234350888 |
| O       | -2.781118199 | 1.468430104 | -1.033259077 |
| H       | 0.225639015 | -0.962449070 | -0.726084050 |
| H       | 1.902694138 | 2.560581184 | 1.100734081 |
| H       | 2.432099176 | -1.602483116 | -1.490371105 |
| H       | 4.126267299 | 1.881007136 | 0.371622026 |
| H       | -1.518957107 | -0.473230032 | 1.321350093 |
| H       | -3.270860234 | -1.539791111 | 1.610051118 |
|   | X            | Y            | Z            |
|---|--------------|--------------|--------------|
| C | 67.8871704   | 0.8871704    | 6.67333583   |
| C | 10.19865253  | 13.50284804  | 6.94685609   |
| C | 10.19865253  | 14.50284804  | 3.59442258   |
| C | 11.862481653 | 13.862481653 | 0.31059495   |
| C | 12.362481653 | 13.862481653 | 0.31059495   |
| C | 11.362481653 | 14.50284804  | 0.31059495   |
| C | 10.9735597   | 13.862481653 | 0.31059495   |
| C | 9.37228875   | 13.862481653 | 0.31059495   |
| C | 9.26228875   | 13.862481653 | 0.31059495   |
| C | 9.15228875   | 14.50284804  | 0.31059495   |
| C | 9.04228875   | 13.862481653 | 0.31059495   |
| N | 15.715534733 | 14.562481653 | 0.31059495   |
| N | 15.549451718 | 10.793451718 | 0.31059495   |
| N | 13.42621066  | 6.395427004  | 0.31059495   |
| C | 10.96932390  | 9.995291420  | 0.31059495   |
| H | 0.072152024  | 12.38845093  | 0.31059495   |
| H | 9.151099548  | 13.57208667  | 0.31059495   |
| H | 0.852924737  | 14.562481653 | 0.31059495   |
| H | 0.852924737  | 14.562481653 | 0.31059495   |
| H | 1.837316852  | 14.40579138  | 0.31059495   |
| N | 15.715534733 | 14.562481653 | 0.31059495   |
| N | 15.549451718 | 10.793451718 | 0.31059495   |
| N | 13.42621066  | 6.395427004  | 0.31059495   |
| C | 10.96932390  | 9.995291420  | 0.31059495   |
| H | 0.072152024  | 12.38845093  | 0.31059495   |
| H | 9.151099548  | 13.57208667  | 0.31059495   |
| H | 0.852924737  | 14.562481653 | 0.31059495   |
| H | 0.852924737  | 14.562481653 | 0.31059495   |
| H | 1.837316852  | 14.40579138  | 0.31059495   |

**Complex 2**

$S_{\text{so}}/F_{\text{so}}$ - Min

|   | X            | Y            | Z            |
|---|--------------|--------------|--------------|
| C | 67.8871704   | 0.8871704    | 6.67333583   |
| C | 10.19865253  | 13.50284804  | 6.94685609   |
| C | 11.862481653 | 13.862481653 | 0.31059495   |
| C | 12.362481653 | 13.862481653 | 0.31059495   |
| C | 11.362481653 | 14.50284804  | 0.31059495   |
| C | 10.9735597   | 13.862481653 | 0.31059495   |
| C | 9.37228875   | 13.862481653 | 0.31059495   |
| C | 9.26228875   | 13.862481653 | 0.31059495   |
| C | 9.15228875   | 14.50284804  | 0.31059495   |
| C | 9.04228875   | 13.862481653 | 0.31059495   |
| N | 15.715534733 | 14.562481653 | 0.31059495   |
| N | 15.549451718 | 10.793451718 | 0.31059495   |
| N | 13.42621066  | 6.395427004  | 0.31059495   |
| C | 10.96932390  | 9.995291420  | 0.31059495   |

S67
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| C    | 20.426675271 | 16.413456383 | 5.657368823 |
| C    | 20.589801482 | 14.046193909 | 6.360187658 |
| C    | 19.420502799 | 11.596913935 | 2.484500181 |
| C    | 19.248348385 | 13.904122200 | 6.045660606 |
| C    | 19.084758371 | 16.247058169 | 5.555958702 |
| C    | 18.519795357 | 10.512286583 | 2.15751260 |
| C    | 18.476803029 | 14.991319813 | 5.646066060 |
| C    | 17.500539595 | 15.662960292 | 1.07511773 |
| C    | 17.345119847 | 9.501660487 | 6.540777671 |
| C    | 17.080621300 | 10.671601768 | 2.476915679 |
| C    | 16.992699925 | 14.618816250 | 1.729749725 |
| C    | 16.995255722 | 14.788947655 | 5.314663833 |
| C    | 16.839129409 | 10.654571665 | 5.947444207 |
| C    | 16.67274702 | 16.763251806 | 0.72698351 |
| C    | 16.499616086 | 8.403712906 | 6.742211584 |
| C    | 16.21565267 | 9.591501789 | 2.256415654 |
| C    | 15.127672633 | 15.88044342 | 5.390987689 |
| C    | 14.536807608 | 16.732652703 | 1.179591387 |
| C    | 14.177113493 | 8.534338215 | 6.33871057 |
| C    | 14.923811227 | 15.630943247 | 1.900128236 |
| C    | 14.83556468 | 9.743454703 | 2.431405473 |
| C    | 14.741213958 | 9.71167599 | 5.748378614 |
| C    | 14.750602764 | 15.717783829 | 5.20732376 |
| C    | 14.25058752 | 7.43960138 | 1.47807807 |
| C    | 14.11894515 | 18.019738298 | 6.131172239 |
| O    | 13.827458400 | 8.599686018 | 2.15303155 |
| C    | 13.784046294 | 16.807880912 | 5.413165391 |
| C    | 12.55682602 | 8.695629424 | 2.59029789 |
| C    | 12.500823299 | 16.783737059 | 4.87979155 |
| C    | 12.156112276 | 6.527836668 | 1.67849723 |
| C    | 12.05417467 | 18.94323464 | 5.78705317 |
| C    | 11.685666543 | 7.64696149 | 2.350996069 |
| C    | 11.62476635 | 17.84132284 | 5.06790866 |
| H    | 16.953651010 | 11.82760150 | 2.895312708 |
| C    | 16.627580094 | 13.591495579 | 5.01040559 |
| C    | 14.305407929 | 10.84417558 | 2.840048507 |
| C    | 14.23386224 | 14.59158365 | 4.84385664 |
| H    | 21.432929042 | 12.36796193 | 2.48387798 |
| H    | 20.952660205 | 8.313454096 | 1.15351882 |
| C    | 20.89667304 | 17.38658325 | 5.78212518 |
| H    | 21.183269724 | 13.96394987 | 6.67486758 |
| C    | 18.988706668 | 12.512617299 | 2.86367083 |
| H    | 18.790798055 | 12.928571432 | 6.11498673 |
| C    | 18.518492233 | 17.11069829 | 5.236291976 |
| H    | 18.53611343 | 8.47184912 | 1.51741211 |
| H    | 18.385632526 | 9.40787448 | 6.32265359 |
| H    | 18.527337334 | 15.66564624 | 0.66884594 |
| H    | 17.601258866 | 13.750276092 | 1.96434274 |
| H    | 17.459716154 | 11.519510327 | 5.76338217 |
| H    | 17.043085429 | 17.612402068 | 0.16289441 |
| H    | 16.866288114 | 7.520208943 | 7.20338147 |
| H    | 16.604252495 | 8.653887420 | 1.92234293 |
| H    | 16.50726790 | 16.845446413 | 5.67741310 |
| H    | 15.262065397 | 7.318954829 | 1.10289680 |
| H    | 15.10054288 | 18.115381906 | 6.58058874 |
| H    | 14.682510156 | 17.549516861 | 0.95092657 |
| H    | 14.484733044 | 7.714281657 | 6.472246164 |
| H    | 13.910458399 | 15.57098321 | 2.271964764 |
| Element | X Coordinate | Y Coordinate | Z Coordinate |
|---------|--------------|--------------|--------------|
| C       | 17.01345259  | 14.784010078 | 5.313074219  |
| C       | 16.85607137  | 10.660685709 | 5.940824573  |
| C       | 16.700397465 | 16.765607137 | 5.940824573  |
| C       | 16.528375753 | 10.86030846   | 5.313074219  |
| C       | 16.230790493 | 16.63418026   | 2.260771744  |
| C       | 16.14918167  | 15.857050563  | 5.313074219  |
| C       | 15.392414025 | 16.734318023  | 1.994087474  |
| C       | 15.20305983  | 8.530630415   | 6.330161273  |
| C       | 14.949762754 | 15.628914593  | 1.994087474  |
| C       | 14.849579100 | 9.750329027   | 2.43834440   |
| C       | 14.762519121 | 9.703630864   | 5.746292026  |
| C       | 14.771345845 | 15.71739836   | 5.192740789  |
| C       | 14.272463335 | 7.43467158    | 1.493244321  |
| C       | 14.15479176  | 18.024583451  | 6.115362423  |
| C       | 13.89454384  | 8.599177717   | 2.16324740   |
| C       | 13.812702909 | 16.87487815   | 5.399273308  |
| C       | 12.574263990 | 8.697371777   | 2.59427630   |
| C       | 12.526623920 | 16.79709308   | 4.872146039  |
| C       | 12.17661246  | 6.528601419   | 1.67847053   |
| C       | 12.09084967  | 18.958785330  | 5.783084793  |
| C       | 11.703621712 | 7.649520045   | 2.355763364  |
| C       | 11.654555604 | 17.854997287  | 5.063968537  |
| O       | 16.710989176 | 11.835301793  | 2.897351311  |
| O       | 16.640185080 | 13.584877247  | 5.019107568  |
| O       | 14.31062949  | 10.84800236   | 2.859369709  |
| O       | 14.28325986  | 14.587100017  | 4.849634569  |
| H       | 21.450502853 | 12.371717096  | 2.471382697  |
| H       | 20.96015777  | 8.30683780    | 1.176138220  |
| H       | 20.913861559 | 17.37394057   | 5.829824491  |
| H       | 21.186129445 | 13.175904385  | 6.69329005   |
| H       | 19.007706999 | 12.524583312  | 2.846432562  |
| H       | 18.801356035 | 12.916300002  | 6.103642745  |
| H       | 18.540340408 | 17.107392572  | 5.265076630  |
| H       | 18.550709298 | 8.471426798   | 1.53706683   |
| H       | 18.409817762 | 9.476675656   | 6.814087750  |
| H       | 18.553585997 | 15.66066893   | 0.682540367  |
| H       | 17.626629872 | 13.759680444  | 1.975482954  |
| H       | 17.472209431 | 11.526855956  | 5.760722536  |
| H       | 17.071475598 | 17.616474283  | 0.18439617   |
| H       | 16.901025886 | 7.517304962   | 7.18043044   |
| H       | 16.618406742 | 8.661886718   | 1.92596427   |
| H       | 16.531742120 | 16.845354460  | 5.652892131  |
| H       | 15.285371543 | 7.316880027   | 1.122382199  |
| H       | 15.139877672 | 18.117585338  | 6.56355809   |
| H       | 14.710858277 | 17.551250573  | 1.00491005   |
| H       | 14.513591376 | 7.707972165   | 6.46214735   |
| H       | 13.934086269 | 15.563213496  | 2.27755350   |
| H       | 13.743359221 | 9.815106720   | 5.401663866  |
| H       | 12.246290822 | 9.592838624   | 3.10887067   |
| H       | 12.225886287 | 15.913977821  | 4.320602447  |
| H       | 11.513276998 | 5.690151924   | 1.489543826  |
| H       | 11.424247923 | 19.80239476   | 5.946341140  |
| H       | 10.649996963 | 17.828198630  | 4.663708391  |
| H       | 10.672333905 | 7.695727666   | 2.678727419  |
| Eu      | 14.902965001 | 12.717684074  | 3.882354952  |

C) antenna meta-Br-PPPDD

$S_{o-Min}$

S70
| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| N    | -4.82692070 | -0.237624926 | -0.242321618 |
| O    | -0.521525357  | 2.684266995 | -0.129237546 |
| O    | -3.433725937  | 2.143473453 | -0.081386852 |
| H    | 0.369666859   | -1.255082300 | 0.104692313 |
| H    | 1.764435733   | 2.765894205 | -0.115862722 |
| H    | 4.091567233   | 1.963567333 | -0.036726663 |
| H    | 4.560814871   | -0.464146884 | 0.113894777 |
| H    | -1.458676769  | -0.465673899 | 0.010946079 |
| H    | -2.880801493  | -1.843073838 | -0.439560600 |
| H    | -5.580247943  | 1.359770308 | 0.294895960 |
| H    | -6.830098124  | -2.716599058 | -0.030843133 |
| H    | -7.423287236  | -0.334587711 | 0.329728598 |
| C    | 0.888100106   | 0.836291626 | -0.013543757 |
| C    | 1.157635696   | -0.533185740 | 0.071367998 |
| C    | 1.976978648   | 1.717084789 | -0.051023921 |
| C    | 2.478280342   | -0.975784896 | 0.116051074 |
| C    | 3.274907578   | 1.262866892 | -0.006349825 |
| C    | 3.551376798   | -0.100577363 | 0.078481759 |
| C    | 0.519842695   | 1.463431226 | -0.071153893 |
| C    | 1.645158467   | 0.584015316 | -0.046961078 |
| C    | -2.988124847  | 1.003810479 | -0.065696334 |
| C    | -3.861077465  | -1.450253421 | -0.250407918 |
| C    | -4.062188675  | -0.095130512 | -0.056278233 |
| C    | -5.395343289  | 0.312859496 | 0.153905472 |
| C    | -6.59444326   | -1.961427473 | -0.035833613 |
| C    | -6.397141090  | -0.615323479 | 0.169003915 |
| Br   | 2.614206186   | -2.509675180 | 0.233172070 |

$S_1(\pi\pi^*)-\text{Min}$

| Atom | X         | Y         | Z         |
|------|-----------|-----------|-----------|
| N    | -5.157386372 | -1.929587137 | -1.201521085 |
| O    | -0.644497047  | 2.484619177 | -1.007937072 |
| O    | -3.048182222  | 1.799005131 | 0.828003059 |
| H    | 0.278058022   | -1.064745075 | 0.650945046 |
| H    | 1.889542136   | 2.622622190 | -0.906062064 |
| H    | 4.128149298   | 1.878783137 | -0.34212025 |
| H    | 4.794323200   | -0.366558027 | 0.743866052 |
| H    | -1.498353109  | -0.543522038 | 0.883782062 |
| H    | -3.313509238  | -1.266674092 | -1.736314127 |
| H    | -5.121607370  | 0.773675056  | 1.541238109 |
| H    | -7.023704505  | -2.449683175 | -0.532206037 |
| H    | -7.096973509  | -0.734981055  | 1.258766088 |
| C    | 0.871620060   | 0.882537061  | -0.195059015 |
| C    | 1.081713080   | -0.405310032  | 0.422379030 |
| C    | 2.032771144   | 1.664031118  | -0.449256032 |
| C    | 2.365228169   | -0.789091058  | 0.743422051 |
| C    | 3.284070234   | 1.251021092  | -0.134591010 |
| C    | 3.502321252   | -0.019685002  | 0.489870304 |
| C    | -0.407741029  | 1.384751700  | -0.539143038 |
| C    | -1.598734117  | 0.443779032  | -0.436593033 |
| C    | -2.872240205  | 0.805852060  | 0.159527012 |
| C    | -4.11095295   | -1.122130083  | -1.033172075 |
| C    | -4.037193289  | -0.134832008  | -0.04389003 |
| C    | -5.137215368  | 0.010356999  | 0.787414058 |
| C    | -6.191984447  | -1.781368130  | -0.379228028 |
| C    | -6.230237448  | -0.822336058  | 0.626750046 |
| Br   | 2.614206186   | -2.509675180  | 1.573452113 |

$T_1(\pi\pi^*)-\text{Min}$
| Element | X         | Y         | Z            |
|---------|-----------|-----------|--------------|
| N       | -4.823693014 | -2.387112294 | -0.062379271 |
| O       | -0.597204911 | 2.719461975 | -0.025229076 |
| O       | -3.423367472 | 2.138611748 | -0.004401225 |
| H       | 0.3728303174 | -1.262199565 | 0.047748002   |
| H       | 1.826642773 | 2.792644944 | -0.042773824  |
| H       | 4.108800629 | 1.957663032 | -0.039628301  |
| H       | 4.569206989 | -0.504754544 | 0.008049383   |
| H       | -1.456790570 | -0.497734570 | 0.023287826   |
| H       | -2.856273313 | -1.867715823 | -0.082021775  |
| H       | -5.635331448 | 1.366782626 | 0.071476378   |
| H       | -6.198768545 | -2.734897411 | -0.03967346   |
| H       | -7.454061274 | -0.336433626 | 0.050474106   |
| O       | 0.866233734  | 0.878645766 | 0.003721767   |
| O       | 1.152366133  | -0.527712052 | 0.029228095   |
| C       | 2.008061662  | 1.736120152 | -0.021491936  |
| C       | 2.461347235  | -0.969739598 | 0.029592036   |
| C       | 3.285785626  | 1.261936119 | -0.01939977   |
| C       | 3.567255555  | -0.123760091 | 0.006896787   |
| O       | 0.596053045  | 1.844217130 | -0.048658799  |
| C       | 0.320878023  | -3.562937257 | 0.154355013   |
| C       | 1.653487119  | -5.62091404 | -0.107380007  |
| Br      | -2.776160751 | -2.866554391 | 0.066626622   |

STC(S1//S0)

| Element | X         | Y         | Z            |
|---------|-----------|-----------|--------------|
| N       | 4.130532298 | -3.389507245 | -0.173113013 |
| O       | 0.596033045 | 1.844217130 | -0.426459029 |
| O       | -0.058363006 | -1.233564090 | 0.402447029 |
| H       | 0.844157063  | 1.663969120 | 3.655928262  |
| H       | 2.812303020  | 0.657161047 | 0.770803058  |
| H       | 4.017191289  | -1.377342099 | -0.02823002   |
| H       | 0.320878023  | -3.562937257 | 0.154355013   |
| H       | 1.653487119  | -5.62091404 | -0.107380007  |
| H       | 4.145273297  | -5.423845389 | -0.30516025   |
| H       | -0.771920056 | 3.269477235 | 0.124187001   |
| H       | -1.238031087 | 5.315461385 | 3.799645273   |
| H       | -1.665291121 | 5.170963372 | 1.36111100    |
| C       | 0.029966001  | 3.603142626 | 3.773093270   |
| C       | 0.293055021  | 2.422828176 | 1.73091124    |
| C       | 0.360989024  | 2.427157174 | 3.121856224   |
| C       | 0.746454051  | 1.538488113 | 0.788665055   |
| C       | 1.712280124  | 0.384269029 | 0.71256050    |
| C       | 1.161169081  | -0.994194069 | 0.34181026   |
| C       | 2.025361144  | -2.221187159 | 0.095345044   |
| C       | 3.400014245  | -2.259721626 | -0.036624003  |
| C       | 1.388180099  | -3.490080250 | 0.058338003   |
| C       | 2.134399153  | -4.651433334 | -0.087338006  |
| C       | 3.521012225  | -4.54711329  | -0.199582015  |
| C       | -0.591651042 | 3.386336246 | 1.157568083   |
| C       | -0.834486058 | 4.526041326 | 3.218403232   |
| Br      | 0.573652041  | 3.797280192 | 5.589104401   |

STC(S1//T1)
N  -5.157386372  -1.929587137  -1.201521085
O  -0.644497047   2.484619177  -1.007937072
O  -3.048512222   1.799005131   0.828003059
H   0.278058022   1.064745075   0.650945046
H   1.889542136   2.622622190  -0.906062064
H   4.128419298   1.878783137  -0.344212025
H   4.479432320  -0.366580277   0.743860052
H  -1.498353109  -0.543522038  -0.883782062
H  -3.313509238  -1.266749092  -1.736314127
H  -5.121607370   0.773675056   1.541238109
H  -7.023704505  -2.449683175  -0.532206037
H  -7.096735099  -0.734981055  1.256766088
C   0.871620060   0.882537061  -0.195059015
C   1.081713080  -0.405310032   0.422379030
C   2.032771144   1.664031118  -0.449256032
C   2.365228169  -0.789091058   0.743422051
C   3.284070234   1.251021092  -0.134591010
C   3.502321252  -0.019685002   0.489870344
C  -0.407741029   1.384757100  -0.539143038
C  -1.598734117   0.443779032  -0.436930333
C  -2.872240205   0.805852060   0.159527012
C  -4.111052959  -1.121300831  -1.031720757
C  -4.307193289  -0.134832008   0.003889003
C  -5.137215368   0.010356999   0.787414058
C  -6.191984444  -1.781368130  -0.379226028
C  -6.230237448  -0.822336058   0.626750046
Br   2.614206186  -2.509675180   1.573452113

Complex 3

S_{0}/F_{0}  = \text{Min}

N   10.467170955  -0.913760365   10.723803770
Br   5.722611413   2.814460505   1.021479972
Br  -0.624051845   3.343579142   5.262129277
Br   0.092835306  -2.423655772   4.050366591
C   11.413930216  -2.156963557   8.922646544
C   11.368521320  -1.782608310   8.109585334
C   10.470678511  -1.602033114   8.032882477
C   9.587273292  -0.422046728   9.908069314
C   9.529207588  -0.723856653   8.518675415
C   9.225110667   0.839523963   0.923523242
C   9.07590955   0.589057343   3.365855340
C   8.673723423   0.114121408   6.320156553
C   8.437933206  -0.104414105   7.687495555
C   8.238354695  -1.504025910   1.303720796
C   7.962198715   0.993520673   4.090155991
C   7.681244650   0.685879751   5.484791193
C   7.096827213   1.924510840   2.001774444
C   6.924056000   1.684515622   3.331412040
O   7.406103432   0.207852415   8.313903999
O   6.550030769   0.955234167   5.868063820
H   12.150727375  -2.856774005   8.575231816
H   12.070895769  -2.180785455   10.943496086
H   10.475144555  -1.892068534   6.998893004
H   10.112241127   0.512439398   1.481940505
H   9.858310608   0.067471703   3.880581812
H   9.640266594  -0.113088060   5.924990828
H   8.883623441   0.280997818   10.308726343
H   8.325493000   1.702954523   0.253298220

S73
H   2.146429956 -2.599695188 14.220611825
H   1.931099938 -0.575907341 5.459304895
H   1.584931714  1.102559880 0.814354557
H   1.715681326 -1.344221895 12.13047074
H   1.565151714  0.378222226 10.94034486
H   1.516204909  2.132573852  6.830770894
H   0.336986422 -0.941663067  5.459304895
H   0.121436008  2.259483960 10.87571584
Eu  5.216407278  1.041429774  7.836869562

Si/Fo-Min
N   10.498828158 -0.895215063 10.741576473
Br  5.728538410  2.840440404  1.011885174
Br -0.591649544  3.330289840  5.233545754
Br  0.061834102 -2.413818171  4.101284942
C   11.43296921  -2.136199356  8.932655741
C   11.38851920  -1.746529126 10.261626737
C   10.494931355 -1.612915819  8.065426248
C   9.59742888  -0.409663067  9.909325111
C   9.540571289  -0.26116150  8.552621417
C   9.249978164  0.869255061  1.988245742
C   9.12422758  -2.413818171  3.33620242
C   8.703513927  0.084454408  6.359806588
C   8.452793610 -0.117837909  7.73064257
C   8.255153697  1.525039708  1.276640891
C   7.944866171  0.985015971  4.037498988
C   7.636184449  0.701462550  5.385309865
C   7.105178413  1.91845341  1.98820404
C   6.92191997  1.685179121  3.30691740
O   7.414264631  0.206592317  8.307356498
O   6.564112975  0.917317368  5.88578626
C   12.175365576 -2.834218205  8.595224317
C   12.10562871 -2.136760453 10.96589993
H   10.492512655 -1.912792236  7.031430805
H   10.140746630  0.556914741  1.470502807
H   9.915994114  0.071507806  3.83427776
H   9.674881496 -0.158272613  5.962055128
H   8.902129241  0.29813824  10.311070143
H   8.352792799  1.728576026  0.22844717
H   6.04110234  2.018542446  3.821773375
N   6.253475150  2.574965983  9.66428149
N   5.333405383 -1.798805732 13.47218768
N   4.68350436  7.145964416  4.49639524
C  -1.405571599  3.54801240  8.016391377
C  -1.204726089  3.08458519  9.363945475
C  -0.404174830  2.99973318  7.120813912
C  -0.037625201  2.47188580  9.08392605
C   7.512871239  4.033396792 11.698796642
C   7.46941340  2.643915293 11.751382044
C   6.908718597  4.681056435 10.635799768
C   6.83299292  1.959499442 10.731245272
C   6.691951482  6.822787490  5.815306016
C   6.292152652  3.927320783  9.642622994
C   6.336276456  5.514022595  6.08744739
C   5.851184122  7.592695447  5.023751564
C   5.155231970  5.006803958  5.538507998
C   5.07918762  1.109106681 12.340519086
C   4.765649245  3.561552157  5.835885322
C   4.370810816  5.860623322  4.774132644
C  4.255073105  -2.318524567  14.104388213
C  3.962048083   2.880362107   4.89587385
C  3.793422371  -0.899345164  11.813243251
C  3.628619859  -0.057346806   10.55376278
C  3.523461153   1.551412913   5.101845769
C  2.950392413  -2.179447859  13.650952385
C  2.432537875  -1.39737601   2.771252299
C  2.14637694   -1.459155405  12.493853497
C  1.59715413   -0.741995533  1.867291037
C  1.854386732   3.051104819  6.934099298
C  0.956097969   2.129168653   8.891994941
C  0.761665572  -2.399646074   7.540313440
C  5.203930474   3.051104819  9.770598003
C  3.832786776   3.821816569   6.111347338
C  3.265279333   1.816500631   8.494543112
H  -2.315619067   3.830914173   7.668390553
H  -1.970893443  -3.58836539   10.078167726
H   8.006233677   4.598771633  12.481940097
H   7.912169669   2.095710550  12.57230204
H   7.608678145   7.244176824  6.20490449
H   6.912179998   5.760057816   10.562045958
H   6.754458887   0.883529263   10.737424273
H   6.968599702   4.876764751   6.693319982
H   5.811060617   4.394582215   8.79266932
H   6.10392337    8.623297721   4.790431142
H   5.930535129  -0.701333949   11.823921153
H   5.350505084  -1.992273342   7.908443769
H   4.537019929  -1.643797021   6.608829077
H   4.460212719  -2.875305607  15.01546280
H   3.612775562   3.414009946   4.035254691
H   3.426531147   5.514599594   4.362772211
H   2.974563415   2.758089662   2.447913474
H   2.134086856  -2.634644489  14.19643823
H   1.935580937  -0.581143042   5.484299593
H   1.500588806   1.130388883   0.85705960
H   1.703620625  -1.347863900  12.124515675
H   1.561772610   0.400991331  10.955720790
H   1.534177509   2.134484552   6.827586691
H   0.245844616  -0.903924463  1.545426309
H   0.10076405   2.277746063   10.859596679
Eu  5.206909277   1.043532677   7.844361362

T/Fo-Min
N  10.502793257  -0.943255165  10.752889785
Br 5.734431915  2.844184502  1.018097175
Br -0.608205744   3.332027341   5.234510574
Br  0.077029506  -2.425154777  4.061241892
C  11.507881530  -2.125724351   8.948251742
C  11.440484325  -1.783307929  10.262048539
C  10.551060585  -1.599007315   8.055376278
C   9.622803491  -0.457343231   9.840768415
C   9.566711486  -0.740262852   8.540149613

S76
O  3.818956173  0.825073058  6.103663542  
O  3.255156233  2.812144531  8.493796612  
H  -2.332703766  3.821018673  7.669207450  
H  -1.985100841  3.351054739  10.743294775  
H  7.998850275  4.598514331  12.501592402  
H  7.897655168  2.097387549  12.585441007  
H  7.597969464  7.250392243  6.217584349  
H  6.90666197  7.650935143  10.579993862  
H  6.750642388  0.886247366  10.743294775  
H  6.961287299  4.886269552  6.899775822  
H  5.806210020  4.403583615  8.807277934  
H  6.105752038  8.633852923  4.800159047  
H  6.975240265  -0.692631562  11.841093553  
H  5.346255786  -1.991374746  7.915974168  
H  4.523882225  -1.654348519  6.618647479  
H  4.414030119  -2.854080704  15.035949890  
H  3.605489600  3.421040547  4.301182889  
H  3.425779748  5.524191800  4.357227815  
H  2.984569015  2.276296261  2.43901876  
H  2.106946353  -2.615038191  14.20641123  
H  1.922626541  -0.516249434  5.466426949  
H  1.548918514  1.127438815  0.827550259  
H  1.687841523  -1.340641949  12.124728272  
H  1.544576713  0.397649429  10.951990900  
H  1.519527311  2.132905852  6.82933690  
H  0.29392532  -0.924320468  1.502080607  
H  0.088617006  2.273507866  10.858145680  
Eu  5.201042574  1.041885475  7.848234463  

S$_3^8$D$_6$ - Min

N  10.534692257  -0.881204164  10.770974476  
Br  5.758588814  2.906354209  1.062419378  
Br  -0.568145840  3.292588035  5.184477771  
Br  0.053534402  -2.420576977  4.104140794  
C  11.530846229  -2.104698752  8.986259046  
C  11.469269926  -1.734251526  10.293020542  
C  10.53673163  -1.596824613  8.087600881  
C  9.647274975  -0.416144131  9.953620114  
C  9.585245289  -0.733506052  8.55798217  
C  9.270959068  0.903657763  1.972557340  
C  9.114517154  0.602156443  3.33055738  
C  8.707763628  0.106757107  6.318079654  
C  8.514263315  -0.155897110  7.763920457  
C  8.28318995  1.587596412  1.297763895  
C  7.978717973  0.983460169  4.011263888  
C  7.715368566  0.662207848  5.442635489  
C  7.134967716  1.974807540  2.005357747  
C  6.95902001  1.698830724  3.328355337  
O  7.437719333  0.198724213  8.356299800  
O  6.565165754  0.901736464  5.83745619  
H  12.293064085  -2.784029400  8.649589220  
H  12.177754678  -2.103228253  11.012461090  
H  10.596323262  -1.911340338  7.058465407  
H  10.15897534  0.595243542  1.450776603  
H  9.897905010  0.054767903  3.822277475  
H  9.678054597  -0.106711106  5.914043527  
H  8.933717545  0.283618420  10.344936345  
H  8.384593606  1.821515733  0.257056718  
H  6.069672037  2.015825645  3.845882977  

S78
|   |   |   |   |
|---|---|---|---|
| N | 6.233034049 | 2.579801786 | 9.684718198 |
| N | 5.285699281 | -1.829739730 | 13.472041467 |
| N | 4.703134038 | 7.136856714 | 4.472190720 |
| C | -1.421728201 | 3.325147237 | 7.954484973 |
| C | -1.238327887 | 3.064146620 | 9.306001270 |
| C | -0.402988231 | 2.973910913 | 7.077202711 |
| C | -0.072900077 | 2.467038287 | 9.766417201 |
| C | 7.492778538 | 4.047740898 | 11.715702241 |
| C | 7.450154036 | 2.652492589 | 11.769793638 |
| C | 6.914306944 | 4.687746437 | 10.649924064 |
| C | 6.814650689 | 1.965983430 | 10.749939374 |
| C | 6.700568382 | 8.166608889 | 5.804166020 |
| C | 6.275372552 | 3.932317984 | 9.659789298 |
| C | 6.342387554 | 5.509297498 | 6.079618140 |
| C | 5.865646320 | 7.584218466 | 5.003676061 |
| C | 5.162539574 | 5.001890161 | 5.542547999 |
| C | 5.030613634 | -1.128232682 | 12.344783890 |
| C | 4.770452243 | 3.556793858 | 5.826507872 |
| C | 4.829005156 | 5.853642024 | 4.756042640 |
| C | 4.201226203 | -3.348881471 | 14.094086514 |
| C | 3.975004384 | 2.866865304 | 4.879547853 |
| C | 3.758888369 | -0.906867964 | 11.815347851 |
| C | 3.602765158 | -0.052331303 | 10.562106359 |
| C | 3.519816952 | 1.543622709 | 5.09476267 |
| C | 2.899213210 | -1.198798760 | 8.036351580 |
| C | 2.411061774 | 1.395429298 | 2.770346000 |
| C | 2.673334690 | -1.466207205 | 12.485303299 |
| C | 2.568974834 | 0.909369665 | 4.074386692 |
| C | 2.376018972 | 0.587283742 | 10.31813241 |
| C | 2.265155862 | 1.481673526 | 9.25340367 |
| C | 1.569113913 | 0.751220853 | 1.87096437 |
| C | 1.845739431 | -0.218191517 | 4.46865324 |
| C | 0.86505161 | -0.384060303 | 2.25002736 |
| C | 1.016150871 | -0.845521059 | 3.55087457 |
| C | 0.938893470 | 2.124838550 | 8.873429373 |
| C | 0.766720757 | 2.385972372 | 7.517285641 |
| O | 5.200412673 | 3.052684619 | 6.927486196 |
| O | 4.988599060 | -1.259755290 | 7.386873433 |
| O | 4.624877830 | 0.046727605 | 9.781601302 |
| O | 3.823164074 | 0.816053660 | 6.104101340 |
| O | 3.254473732 | 1.820858292 | 8.501185911 |
| H | -2.331017966 | 3.788807072 | 7.589649646 |
| H | -2.017984043 | 3.334175742 | 10.007125120 |
| H | 7.983124073 | 4.607434132 | 12.499680098 |
| H | 7.989976667 | 2.105767351 | 12.591549608 |
| H | 7.61494250 | 7.239080281 | 6.198256144 |
| H | 6.895140395 | 5.766511714 | 10.575234061 |
| H | 6.742915485 | 0.888161263 | 10.756808073 |
| H | 6.971968801 | 4.873976749 | 6.691694884 |
| H | 5.793750716 | 4.398531718 | 8.809781836 |
| H | 6.127936039 | 8.613091818 | 4.770582246 |
| H | 5.87996026 | -0.720068152 | 11.835290352 |
| H | 5.349406094 | -1.990183642 | 7.925211973 |
| H | 4.543967825 | -1.659405915 | 6.615437574 |
| H | 4.39032918 | -2.915381311 | 15.000818077 |
| H | 3.624901960 | 3.407025497 | 4.019852490 |
| H | 3.438326746 | 5.508104594 | 4.34897413 |
| H | 2.94967610 | 2.275488862 | 2.446129877 |
| H | 2.077963649 | -2.649459898 | 14.176936218 |
|      |      |      |      |      |      |
|------|------|------|------|------|------|
|      |      |      |      |      |      |
| H    | 1.935142038 | -0.592819941 | 5.481234593 |
| H    | 1.463289205 | 1.135680481 | 0.863940561 |
| H    | 1.664990818 | -1.34516497 | 12.11725874 |
| H    | 1.533940311 | 0.414201331 | 10.957014088 |
| H    | 1.544914611 | 2.122863153 | 6.81836591 |
| H    | 0.216044141 | -0.89828764 | 1.554762811 |
| H    | 0.051044903 | 2.77798762 | 10.82605777 |
| Eu   | 5.193811573 | 1.040610873 | 7.856923564 |

Complex 4

$S_0^2/F_0^2$ – Min

|      |      |      |      |      |      |
|------|------|------|------|------|------|
|      |      |      |      |      |      |
| N    | 19.166281180 | 10.614148464 | 6.812805988 |
| Br   | 12.079645270 | 7.33965826 | 7.25673124 |
| Br   | 21.825433570 | 14.54359246 | 0.355137027 |
| Br   | 13.317953557 | 12.10936973 | -5.61934505 |
| C    | 20.200350855 | 11.27936981 | 6.36886860 |
| C    | 20.339044633 | 11.69770564 | 5.04072536 |
| C    | 19.337250189 | 11.39970821 | 4.15883900 |
| C    | 18.185320807 | 10.36430942 | 5.94877329 |
| C    | 18.201076208 | 10.7116970 | 4.61256502 |
| C    | 17.102073933 | 10.36233944 | 3.62775216 |
| C    | 15.835843383 | 9.98776211 | 4.09332919 |
| C    | 14.743177661 | 9.69283049 | 3.22512533 |
| C    | 13.426301667 | 9.26021266 | 3.84124775 |
| C    | 13.364954863 | 8.60219519 | 5.04413826 |
| C    | 12.222616580 | 9.54137158 | 3.15363028 |
| C    | 12.119040722 | 8.23555293 | 5.57340003 |
| C    | 11.009568990 | 9.17863146 | 3.69119176 |
| C    | 10.95008486 | 8.50708173 | 4.92858585 |
| O    | 17.442781853 | 10.43008463 | 2.44270387 |
| O    | 14.750759162 | 9.75848830 | 1.99650604 |
| H    | 20.973401207 | 11.49668152 | 7.08484708 |
| H    | 21.216480126 | 12.23276448 | 4.72688138 |
| H    | 19.39773698 | 11.68523563 | 3.12416192 |
| H    | 17.364513648 | 9.77717880 | 6.35759557 |
| H    | 15.637664523 | 10.29893324 | 5.14277737 |
| H    | 14.25821312 | 8.35757160 | 5.83422699 |
| H    | 12.27262381 | 10.06472642 | 2.21961836 |
| H    | 10.094930326 | 9.41096378 | 3.17649302 |
| H    | 10.005859719 | 8.22293909 | 5.35192608 |
| N    | 22.438834517 | 11.09644400 | 1.06293777 |
| N    | 18.290876216 | 7.70041245 | 1.46108800 |
| N    | 14.045994409 | 8.73984352 | -1.36774820 |
| N    | 10.736944770 | 12.36906888 | -1.28416129 |
| C    | 23.405597583 | 11.30853114 | 0.12998841 |
| C    | 23.165196168 | 11.34936761 | -1.24100059 |
| C    | 21.89697272 | 11.17486060 | -1.76940223 |
| C    | 21.18801523 | 10.93008418 | 0.56943629 |
| C    | 20.844168301 | 10.96159219 | -0.78519685 |
| C    | 20.62482382 | 7.21447618 | 1.27942189 |
| C    | 20.697114867 | 7.00410250 | 2.65034893 |
| C    | 20.051023143 | 15.11939639 | -0.10681710 |
| C    | 19.415608899 | 7.554903042 | 0.70507205 |
| C    | 19.377320994 | 10.75263797 | -1.15444463 |
| C    | 19.843654828 | 16.39127780 | -0.62346843 |
| C    | 19.544830707 | 7.12350615 | 3.41690248 |
| C    | 18.93958261 | 11.17412280 | -2.39837297 |
| C    | 19.015857668 | 14.21644762 | 0.05332140 |
| Element | X (Å) | Y (Å) | Z (Å) |
|---------|-------|-------|-------|
| C       | 18.353 | 7.461 | 9023 | 2.80449001 |
| C       | 18.551 | 16.745 | 10603 | -0.987418669 |
| C       | 17.945 | 1.584 | 6032 | -5.266569778 |
| C       | 17.594 | 5.266 | 569778 | 8902497 |
| C       | 17.130 | 1.652 | 281080 | 0.792849555 |
| C       | 17.732 | 14.562 | 607249 | -0.342944524 |
| C       | 16.888 | 13.456 | 16356 | -0.232990419 |
| C       | 16.020 | 12.099 | 074071 | -6.63531776 |
| O       | 18.630 | 10.174 | 72632 | -2.730765598 |
| O       | 17.056 | 12.917 | 81248 | 999944 |
| O       | 16.908 | 11.406 | 72825 | -3.82654973 |
| O       | 15.225 | 11.903 | 7252156 | -5.51396589 |
| O       | 14.490 | 12.624 | 997309 | -0.76569057 |
| O       | 13.973 | 8.772 | 184132 | -2.730765598 |
| O       | 13.111 | 9.013 | 252150 | -2.634693987 |
| O       | 12.884 | 8.894 | 743639 | -3.82654973 |
| O       | 12.008 | 8.042 | 81775 | 0.84653625 |
| C       | 11.590 | 9.013 | 252150 | -2.634693987 |
| C       | 11.667 | 8.965 | 15944 | -1.249342791 |
| C       | 11.588 | 13.999 | 82407 | -2.861117804 |
| C       | 10.560 | 10.509 | 925455 | -1.988368543 |
| C       | 10.217 | 8.491 | 147310 | -0.720457452 |
| C       | 9.692 | 11.444 | 230235 | -0.28707862 |
| C       | 8.416 | 11.424 | 68124 | 0.51148037 |
| C       | 23.986 | 11.499 | 96927 | -1.929689041 |
| C       | 21.627 | 11.182 | 826906 | -2.77071899 |
| C       | 21.498 | 7.175 | 16313 | 0.648670346 |
| C       | 21.641 | 6.743 | 3028183 | 3.115887026 |
| C       | 20.396 | 10.746 | 761373 | 1.287941794 |
| C       | 20.670 | 17.082 | 157331 | -0.73959453 |
| C       | 19.615 | 11.647 | 825237 | -3.07965572 |
| C       | 19.266 | 7.736 | 325355 | -0.34464525 |
| C       | 19.558 | 6.956 | 81603 | 4.486188321 |
| C       | 19.180 | 13.233 | 90750 | 0.46988073 |
| C       | 19.017 | 11.452 | 410424 | -5.18905874 |
| C       | 18.034 | 12.075 | 823970 | -7.35252130 |
| C       | 18.362 | 17.730 | 115976 | -1.38100299 |
| C       | 17.408 | 7.560 | 717446 | 3.323577639 |
| C       | 16.516 | 16.137 | 798561 | -1.17172586 |
| C       | 15.580 | 12.371 | 324590 | -7.587690547 |
| C       | 15.159 | 14.597 | 523052 | -1.21501386 |
| C       | 15.131 | 11.405 | 969220 | -3.424987246 |
| C       | 14.924 | 8.665 | 286925 | -3.231865332 |
| C       | 13.693 | 14.415 | 456635 | -2.802417203 |
| C       | 12.738 | 8.893 | 376342 | -4.46496732 |
| C       | 13.060 | 7.555 | 82428 | 0.42839713 |
| C       | 12.160 | 11.548 | 970132 | -0.017264604 |
| C       | 11.376 | 14.718 | 861157 | -3.641442961 |
| C       | 10.631 | 9.113 | 863255 | -3.130595126 |
| C       | 10.778 | 9.033 | 954850 | -0.634419846 |
| C       | 9.546 | 13.364 | 123059 | -2.659519089 |
| Eu      | 16.472 | 10.178 | 946235 | 0.304313622 |

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| Atoms | X      | Y      | Z      |
|-------|--------|--------|--------|
| N     | 19.17235680 | 10.63109683 | 6.844236391 |
| Br    | 12.053395168 | 7.404248835 | 7.32699330 |
| Br    | 21.818326471 | 15.53200446 | 0.35837426 |
| Br    | 13.134346060 | 12.117322272 | -5.62139406 |
| C     | 20.211172756 | 11.28792913 | 6.40293563 |
| C     | 20.361282666 | 11.69289340 | 5.07045064 |
| C     | 19.367821293 | 11.40045809 | 4.17792402 |
| Br    | 18.195774101 | 10.351274445 | 5.97631852 |
| Br    | 18.224162511 | 10.708594771 | 4.63566523 |
| Br    | 17.148137236 | 10.36235947 | 3.64938682 |
| C     | 15.828028238 | 9.986755119 | 4.09885797 |
| C     | 14.671704585 | 9.627192209 | 3.22882093 |
| C     | 13.421896668 | 9.239776965 | 3.85099607 |
| Br    | 13.340597961 | 8.627771853 | 3.15778029 |
| C     | 13.340597961 | 8.627771853 | 3.15778029 |
| C     | 12.095578688 | 7.826124988 | 5.63011730 |
| C     | 10.982112899 | 7.14070959 | 3.71560886 |
| C     | 10.918027087 | 7.521538913 | 4.98453195 |
| O     | 17.460261451 | 10.429612351 | 2.47054478 |
| O     | 14.740173363 | 9.814010805 | 1.98032941 |
| C     | 22.421770614 | 11.107547098 | 1.06854417 |
| N     | 18.291658818 | 7.703916451 | 1.43595540 |
| N     | 14.071490412 | 8.759529228 | -1.37729979 |
| N     | 10.738873875 | 12.355218688 | -1.30491296 |
| C     | 23.392928285 | 11.378287174 | 0.13991480 |
| C     | 23.157391685 | 11.357450313 | -1.23397889 |
| C     | 21.864414722 | 11.181039504 | -1.70493422 |
| C     | 21.174371222 | 10.9378564866 | 0.56670545 |
| C     | 20.835469107 | 10.96681387 | -0.78783538 |
| C     | 20.62385658 | 7.200875315 | 1.24364489 |
| C     | 20.698325290 | 6.981878002 | 2.61074769 |
| C     | 20.044286441 | 15.113208789 | -0.70470109 |
| C     | 19.413872695 | 7.561362944 | 0.67378651 |
| C     | 19.393596969 | 10.75507877 | -1.15696885 |
| C     | 19.835722225 | 16.38411827 | -0.62529584 |
| C     | 19.546304106 | 7.094796098 | 3.38077734 |
| C     | 18.935273265 | 11.177110003 | -2.40104657 |
| C     | 19.009205070 | 14.209018520 | 0.04766405 |
| C     | 18.355306222 | 7.442246334 | 2.77575589 |
| C     | 18.542903632 | 16.73243506 | -0.99187076 |
| C     | 17.947357889 | 11.58659637 | -5.26439807 |
| C     | 17.589261163 | 10.989068269 | -2.75105200 |
| C     | 17.396195950 | 11.93861260 | -6.49048369 |
| C     | 17.725735473 | 14.550091345 | -0.35125462 |
| C     | 17.499428957 | 15.825756739 | -0.86834026 |
| C     | 17.128541633 | 11.395223218 | -4.15403499 |
| C     | 16.683285202 | 13.441633667 | -0.24417621 |
| C     | 16.025286953 | 12.105936272 | -6.63679978 |
| C     | 15.759234322 | 11.560705733 | -4.29343511 |

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