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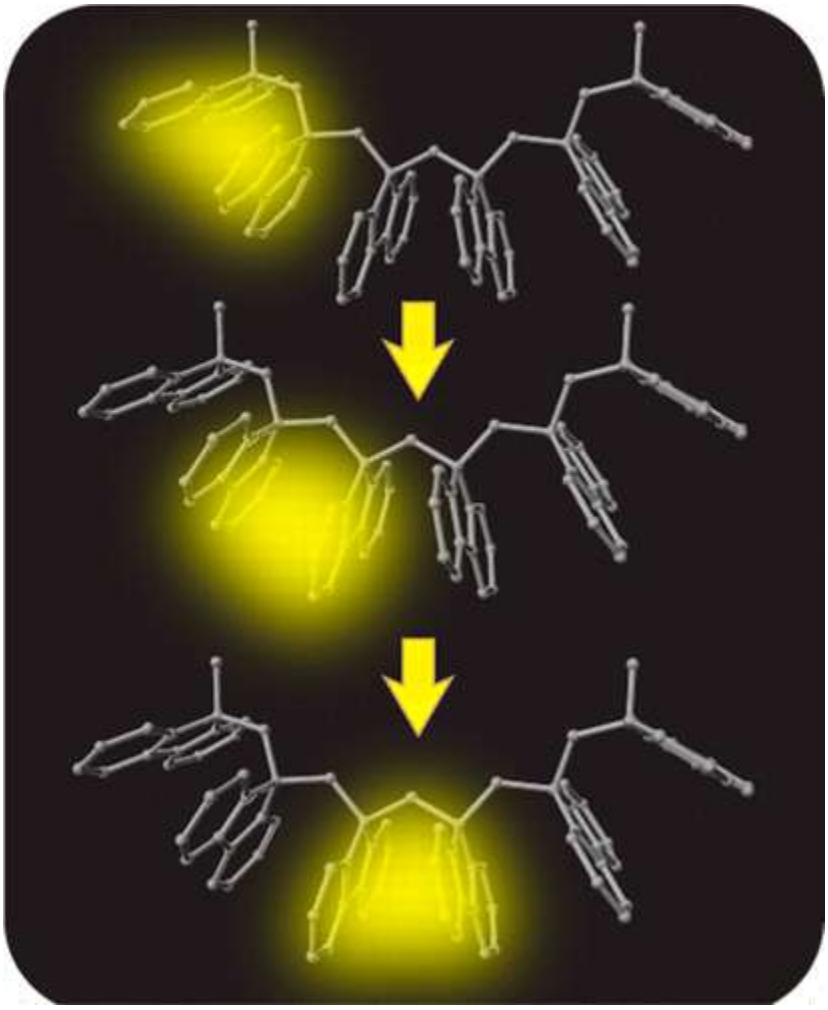
Abstract



Understanding the mechanisms of long-range energy transfer through polychromophoric assemblies is critically important in photovoltaics and biochemical systems. Using a set of cofacially arrayed polyfluorenes (F*n*), we investigate the mechanism of (singlet) exciton delocalization in π-stacked polychromophoric assemblies. Calculations reveal that effective stabilization of an excimeric state requires an ideal sandwich-like arrangement; yet surprisingly, emission spectroscopy indicates that exciton delocalization is limited to only two fluorene units for all *n*. Herein, we show that delocalization is determined by the interplay between the energetic gain from delocalization, which quickly saturates beyond two units in larger F*n*, and an energetic penalty associated with structural reorganization, which increases linearly with *n*. With these insights, we propose a hopping mechanism for exciton transfer, based upon the presence of multiple excimeric tautomers of similar energy in larger polyfluorenes ($n \geq 4$) together with the anticipated low thermal barrier of their interconversion.

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The underlying mechanisms of energy and electron transport through polychromophoric assemblies continue to attract much attention in the field of organic electronics and photovoltaics. We have recently introduced covalently linked cofacially arrayed polyfluorenes containing multiple fluorenes (F2–F6, Figure 1A) that serve as models for the study of charge/energy transfer in π-stacked arrays.[1-4] The cofacially juxtaposed fluorene moieties in F2–F6 are rigidly held in close van der Waals contact with only limited libration of fluorenes along their long axes, as demonstrated by NMR spectroscopy and X-ray crystallography (Figure 1A).[1,5]

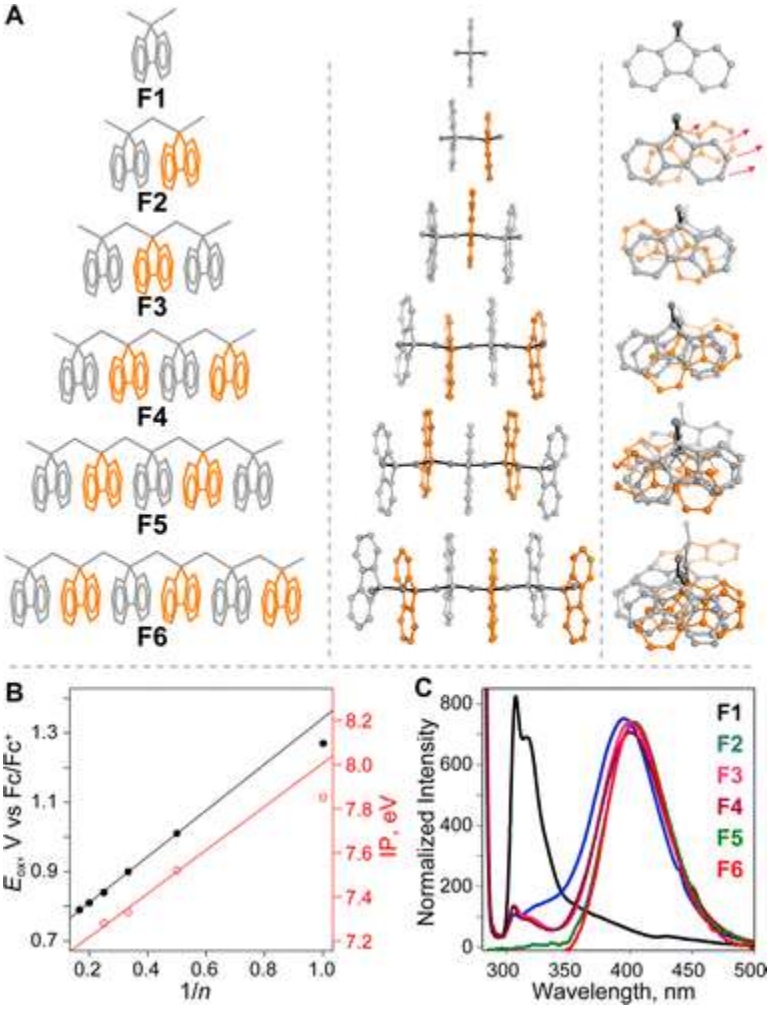

Figure 1. (A) Structures and naming scheme of F1–F6, two views of minimized structures [B1LYP-40/6-3-G(d)+PCM(CH_2Cl_2)] of F1–F6, and representation of the libration of fluorene moieties with red arrows on the example of F2. (B,C) P lot of E_{ox1} values (black axis) and IPs (red axis) vs 1/*n* (B)[1,4] and normalized emission spectra

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(λ_{exc} = 280 nm) of F1–F6 in CH_2Cl_2 at 22 °C (C). Note that the relative emission intensity of F1 was ~10 times higher than that of F2–F6.

The effective electronic coupling among the fluorenes in F2–F6 was demonstrated by the observation that their (vertical) ionization potentials in the gas phase and (adiabatic) oxidation potentials in solution decrease with increasing number of fluorenes (*n*) and follow a 1/*n* trend (Figure 1B).[1,4] Moreover, the delocalization of a hole over multiple fluorene units in F2–F6 was further evidenced in the electronic spectra of their cation–radicals, where the intervalence charge-resonance transition shifted red (to longer wavelength) and intensified with the increasing number of fluorene units (Figure S1 in the SI).

Despite the effective delocalization of the hole in F2–F6, their emission spectra were found to be identical with a broad Gaussian-shaped band at 395 ± 3 nm.[1,4,6] By comparison with the emission spectrum of monomeric F1, which shows a single structured band at 315 nm (Figure 1C), the Gaussian band at 395 nm for F2–F6 can be readily assigned to emission from an excited dimer (or excimer).[7] The observation of nearly identical emission spectra of F2–F6 (Figure 1C) suggests that the exciton most likely resides only over two fluorene moieties, in contrast with the hole in the corresponding cation–radicals (Figure 1B and Figure S1 in the SI).

The central question we address here is why, unlike the hole, is the exciton localized only onto two units? We will also examine whether the exciton occupies the central or outer fluorene units in higher F*n* and probe whether the exciton is dynamic and can migrate along the cofacially juxtaposed π-array and, if so, by what means. In order to address these questions, we undertake a detailed computational study of various polyfluorenes (Figure 1A) in the ground (S_0) and first excited (S_1) states using density functional theory (DFT) and time-dependent DFT (TD-DFT) calculations. We will show that formation of an excimeric state has a stringent requirement of structural/conformational reorganization, which limits the delocalization of the exciton beyond two units in F*n*, as the concomitant reorganization penalty outweighs the energetic benefits of additional delocalization.

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We performed electronic structure calculations of the ground and excited states of F1–F6 using (TD-)DFT calculations with a modified B1LYP-40 density functional, extensively utilized for the accurate description of electronic structures of ion–radicals of different classes of π-conjugated molecular wires in their ground and excited states.[8-11] Additionally, we performed calculations with benchmarked standard density functionals (PBE0, ωB97X-D) and obtained comparable results (details in sections S3 and S4 in the SI).

A close examination of the electronic structures of F1 in its ground (S_0) and first excited (S_1) states shows that dramatic bond length changes accompany electronic excitation (Figure 2). For example, the central C–C bond (*a*) contracts from 1.467 to 1.387 Å (i.e., by 8.0 pm), while the aromatic bonds of similar length (i.e., ~1.39 Å) in the S_0 state undergo elongation (by 5.5, 5.0, 1.7, and 2.4 pm for *b*, *g*, *d*, and *e*, respectively) and contraction (by 1.7 and 2.4 pm for *c* and *f*, respectively), leading to a quinoidal distortion of F1 in the S_1 state. For details, see Figure 2A and Tables S2 and S3 in the SI.

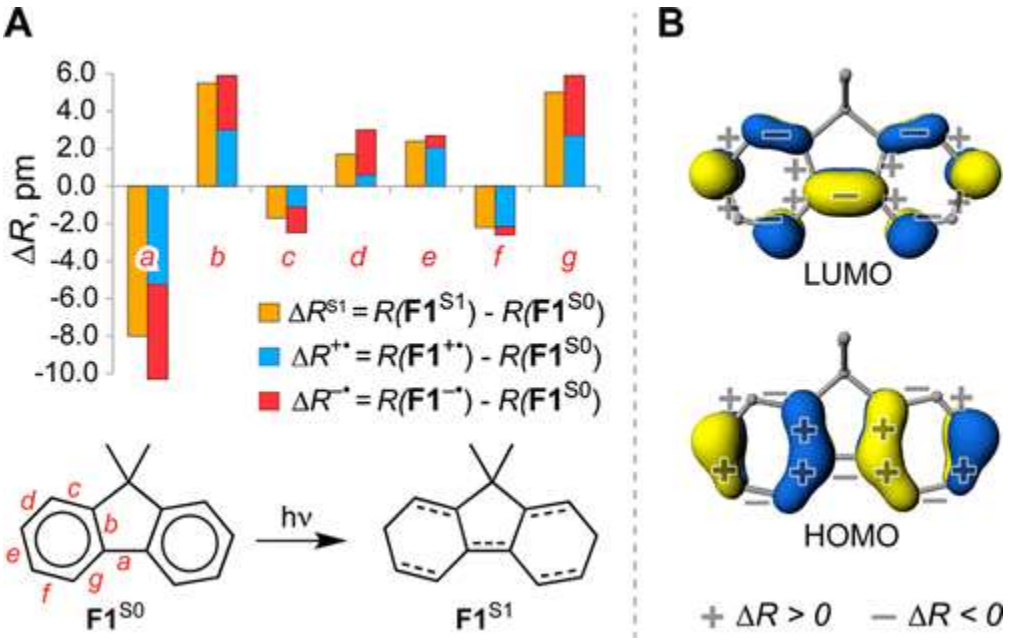

Figure 2. (A) Bar plots showing bond length changes due to the $S_0 \rightarrow S_1$ excitation of F1 as compared with the combined effect of the similar bond length changes due to the oxidation and reduction of F1 [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] and cartoon representation of the structural changes accompanying the excitation of fluorene from the ground to the first excited state. (B) Depiction of the HOMO and LUMO of F1, shown together with the sign of the excitation-induced bond length changes.

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The bond length changes observed in the electronically excited $F1^{S1}$ were significantly larger than our earlier observations of the experimental bond length changes in the X-ray structures of a number of different polycyclic aromatic cation–radicals or anion–radicals.[12-17] However, when we compared the bond length changes in F1 cation– and anion–radicals [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] with $F1^{S1}$, the exciton-induced bond length changes in $F1^{S1}$ were found to be an approximate sum of the changes in $F1^{+\bullet}$ and $F1^{-\bullet}$, that is, $\Delta R^{S1} \approx \Delta R^{+\bullet} + \Delta R^{-\bullet}$ (Figure 2A).

Analysis of the X-ray structures of several neutral electron donors (or acceptors) and their cation (or anion) radicals[12-17] together with DFT calculations[10,18,19] showed that the 1*e*-oxidation (or reduction)-induced bond length changes in cation (or anion) radicals can be predicted by the disposition of the nodal arrangement of the HOMO (or LUMO).[10,12-19] For example, upon 1*e* oxidation of an electron donor, bonds aligned with bonding lobes of the HOMO undergo elongation, while the bonds aligned with antibonding lobes undergo contraction. In contrast, upon 1*e* reduction of an electron acceptor, bonds aligned along bonding lobes of the LUMO undergo contraction, while bonds aligned with antibonding lobes undergo elongation. Interestingly, the nodal arrangement and disposition of the HOMO and LUMO in F1 (Figure 2B) is such that both oxidation- and reduction-induced bond length changes would lead to elongation and contraction of the same bonds. As the observed bond length changes in $F1^{S1}$ are found to be the sum of the bond length changes in the F1 cation–radical and anion–radical, the excited state of F1 (i.e., promotion of an electron from the HOMO to LUMO) accommodates bond length changes arising from the simultaneous formation of cation–radical and anion–radical states (or an electron–hole pair). Moreover, the observed geometrical reorganization in $F1^{S1}$ is consistent with the analysis of electron densities of F1 in its ground, excited, oxidized, and reduced states using a frozen orbital approximation; see section S5 in the SI.

An excited molecule associates with its ground-state counterpart to form an excimer due to the resonance stabilization of the exciton.[20] In the case of F2, the covalently linked cofacially π-stacked fluorene moieties allow spontaneous formation of the excimeric state. Indeed, the calculated geometry of the optimized excited state $F2^{S1}$ (Figure 3A)

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shows that the bond length changes within the fluorene units were equally distributed and were half of that in $F1^{S1}$, suggesting that the exciton is evenly delocalized onto both fluorene moieties (compare Figures 2A and 3A; also compare Tables S2–S5 in the SI). In addition to the bond length changes, the effective delocalization of the exciton in $F2^{S1}$ results in an eclipsed sandwich-like arrangement of the fluorene moieties with an interplanar angle of ~18°, resulting in contacts among the fluorene carbons as close as 3.0–3.2 Å (Figure 3A).

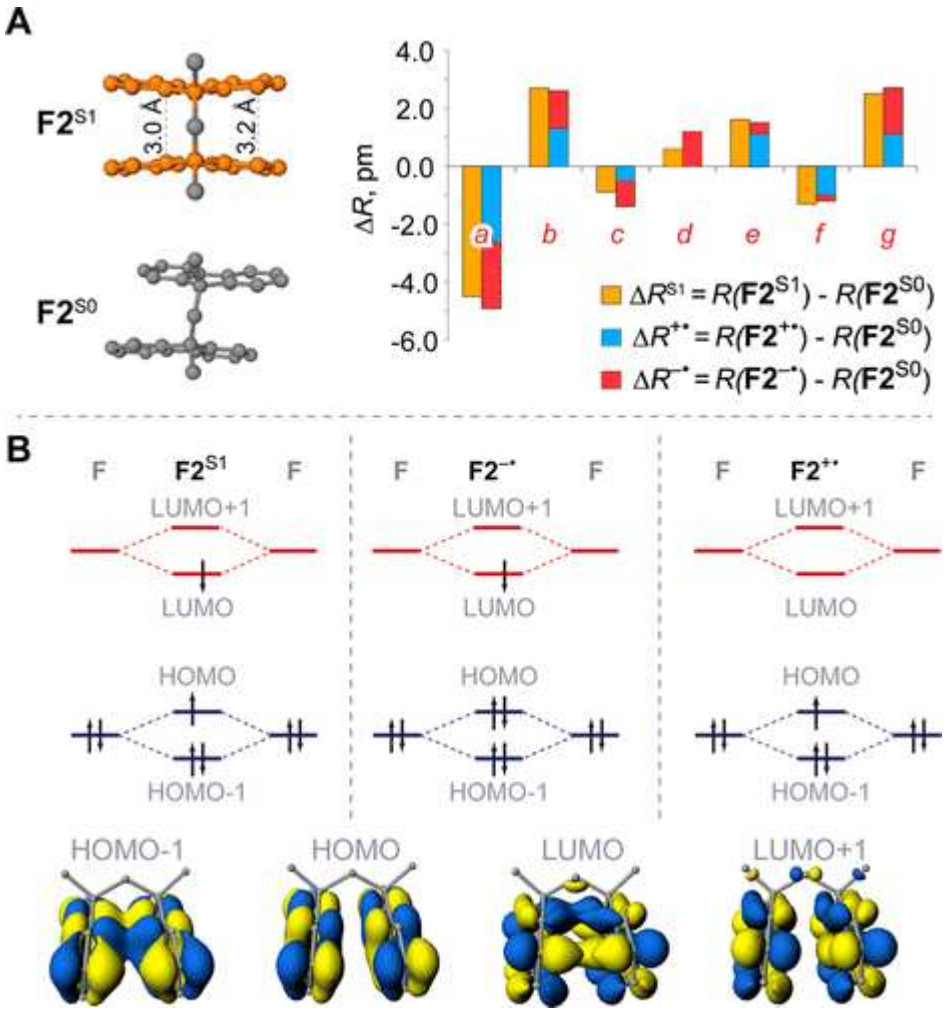

Figure 3. (A) Bar plots showing excitation-induced bond length changes in F2 as compared with the combined effect of the bond length changes due to its oxidation and reduction [B1LYP-40/6-31G(d)+PCM (CH_2Cl_2)]. Note that labeling of bonds in fluorene units corresponds to the structure shown in Figure 2A. (B) Molecular orbital picture of the $S_0 \rightarrow S_1$ excitation, reduction, and oxidation of F2 as well as plots of the relevant molecular orbitals.

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The observation of a close sandwich-like arrangement of the fluorenes in $F2^{S1}$ and complete delocalization of the exciton suggest an effective electronic coupling (V_{ab}) among the fluorenes, which, in turn, demands effective electronic coupling between HOMOs (β_{HOMOs}) and LUMOs (β_{LUMOs}) of the monomeric units, that is, $V_{ab} \approx \beta_{HOMOs}\beta_{LUMOs}$.[21,22] According to the well-known Mulliken approximation,[21,23] coupling between any two orbitals is proportional to the overlap integral. Excimeric coupling V_{ab} will depend on both the LUMO–LUMO and HOMO–HOMO overlaps,[24] whereas the coupling in ion–radicals is proportional to either the HOMO–HOMO or LUMO–LUMO overlap. The product of the HOMO–HOMO/LUMO–LUMO overlap integrals in the excimer will decrease much more rapidly upon displacement of excimeric partners from the ideal sandwich-like arrangement[22,24,25] as compared to the HOMO–HOMO or LUMO–LUMO overlap integrals in cation–radical and anion–radical dimers.[12] Indeed, a simple analysis of the molecular orbital diagram of F2 clearly shows that overlap among the frontier orbitals allows efficient bonding between the monomer units in $F2^{S1}$, which is roughly twice larger than that in $F2^{-\bullet}$ or $F2^{+\bullet}$ alone (Figure 3B).

Consistent with the observation of nearly identical emission spectra of F2–F6 (Figure 1C), optimization of the excited state of higher homologues, that is, $F3^{S1}$ and $F4^{S1}$, showed that the exciton is indeed localized onto only two fluorene moieties in both molecules. For example, the excitation-induced bond length changes in both $F3^{S1}$ and $F6^{S1}$ were localized onto a pair of fluorenes that adopted a close (eclipsed) sandwich-like arrangement akin to that found in $F2^{S1}$ (Figure 4A and section S4 in the SI).

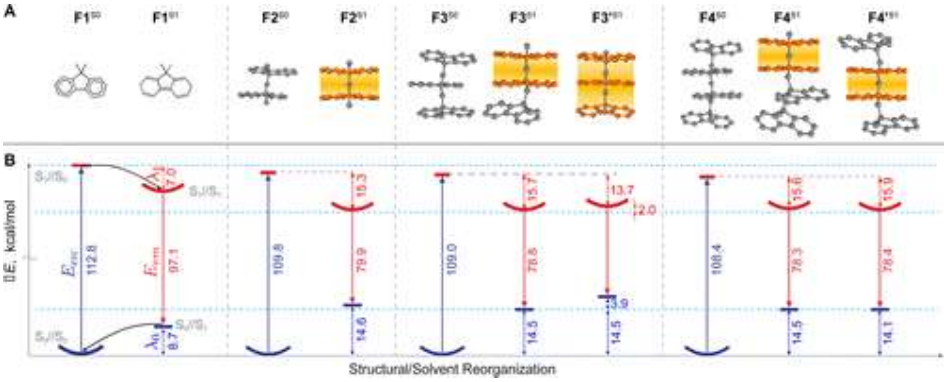

Figure 4. (A) Structures of F1–F4 in their ground (S_0) and first excited (S_1) states [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] with hydrogens omitted for clarity. (B) Energetic

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diagrams of the excitation/emission cycle of F1–F4, where exciton was localized onto two units. Additionally, in F3, full exciton delocalization was enforced by the imposing fully eclipsed conformation of all three fluorenes.

Unlike $F2^{S1}$ and $F3^{S1}$, $F4^{S1}$ can exist in two distinct valence tautomers where the exciton is localized either onto two central fluorenes ($F4^{S1}$) or onto a central and an adjacent terminal fluorene ($F4'^{S1}$),(26) Figure 4A. Comparison of the energies of optimized $F4^{S1}$ and $F4'^{S1}$ showed that they are nearly isoenergetic and differ in energy by only 0.3 kcal/mol (vide infra).[26] The energetic diagrams depicting the absorption–emission cycle of F1–F4 are shown in Figure 4B. A comparison of the electronic energies of the vertically excited state ($S_1//S_0$) and geometrically relaxed excited state ($S_1//S_1$) of $F1^{S1}$–$F4^{S1}$ directly provides the exciton stabilization energy (i.e., $\lambda_1 = E_{S1//S0} - E_{S1//S1}$), whereas the difference in the ground-state electronic energies of $F1^{S0}$–$F4^{S0}$ at the relaxed ($S_0//S_0$) and excited-state ($S_0//S_1$) geometries constitutes the reorganization penalty (i.e., $\lambda_0 = E_{S0//S1} - E_{S0//S0}$) for the accommodation of the exciton (Figure 4B).

As expected, stabilization of the excimeric state in F2–F4 (λ_1 = 15.6 ± 0.3 kcal/mol) is ~8.5 kcal/mol larger than stabilization of the exciton in F1 (λ_1 = 7.0 kcal/mol) due to resonance interactions. The increase in reorganization penalty for the accommodation of the exciton onto two fluorenes in F2 (λ_0 = 14.6 kcal/mol) vs one fluorene in F1 (λ_0 = 8.7 kcal/mol) is also understandable, given that the structural reorganization in F1 is limited to only bond length changes in a single fluorene, whereas F2 undergoes additional geometrical reorganization leading to an eclipsed sandwich-like arrangement.[27] Homodesmic analysis of the reorganization penalty (see section S6 in the SI) shows that the energy required for the bond length changes distributed over one fluorene in F1 and two fluorenes in F2 is nearly identical (9.0 and 8.7 kcal/mol), and the remaining reorganization energy for F2, that is, ~5.6 kcal/mol, is responsible for the conformational reorganization in an eclipsed sandwich-like arrangement of $F2^{S1}$. The calculated reorganization penalty of ~14.5 kcal/mol for $F3^{S1}$ and $F4^{S1}$, which is similar to that in $F2^{S1}$, further attests that the exciton localizes only onto two fluorenes.

Calculations of isomeric $F3'^{S1}$, where all three fluorenes are enforced in an eclipsed π-stacked arrangement, show that the exciton is distributed on all three units with a 1:2:1 ratio as judged by the

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bond length changes within each fluorene (Table S8 in the SI; as well as by the analysis of the molecular orbitals involved in the $S_0 \rightarrow S_1$ transition). Despite the increased delocalization of the exciton in $F3'^{S1}$, its stabilization energy (λ_1 = 13.7 kcal/mol) is 2.0 kcal/mol less than that of $F3^{S1}$ (λ_1 = 15.7 kcal/mol), where the exciton is delocalized onto two fluorenes (Figure 4B). This is not surprising based on the additional reorganization penalty of 3.9 kcal/mol[28] required to geometrically reorganize three fluorenes into an eclipsed multidecker sandwich-like structure.[29]

To gain further insight into the size dependence of the interplay between the energetic gain from the exciton delocalization and the energetic penalty needed for structural reorganization in terms of bond length changes and geometrical reorganization for an optimized sandwich-like arrangement of interacting chromophores in larger F*n*, we carried out additional single-point TD-DFT calculations on a representative polyfluorene F9, as follows.

Single-point (TD-)DFT calculations were performed for a series of F9 molecules in both the ground and excited states, where an increasing number of fluorenes (*k*) were arranged in eclipsed sandwich-like arrangement akin to that in $F2^{S1}$ while the internal structural parameters for all fluorenes were fixed at the values corresponding to parent $F1^{S0}$ (see section S7 in the SI for details). A compilation of various F9 excited-state structures showing the transition densities of the $S_0 \rightarrow S_1$ excitation in Figure 5A demonstrates that exciton delocalization extends to all fluorenes (*k* = 2–9), which are arranged in an eclipsed sandwich-like arrangement.

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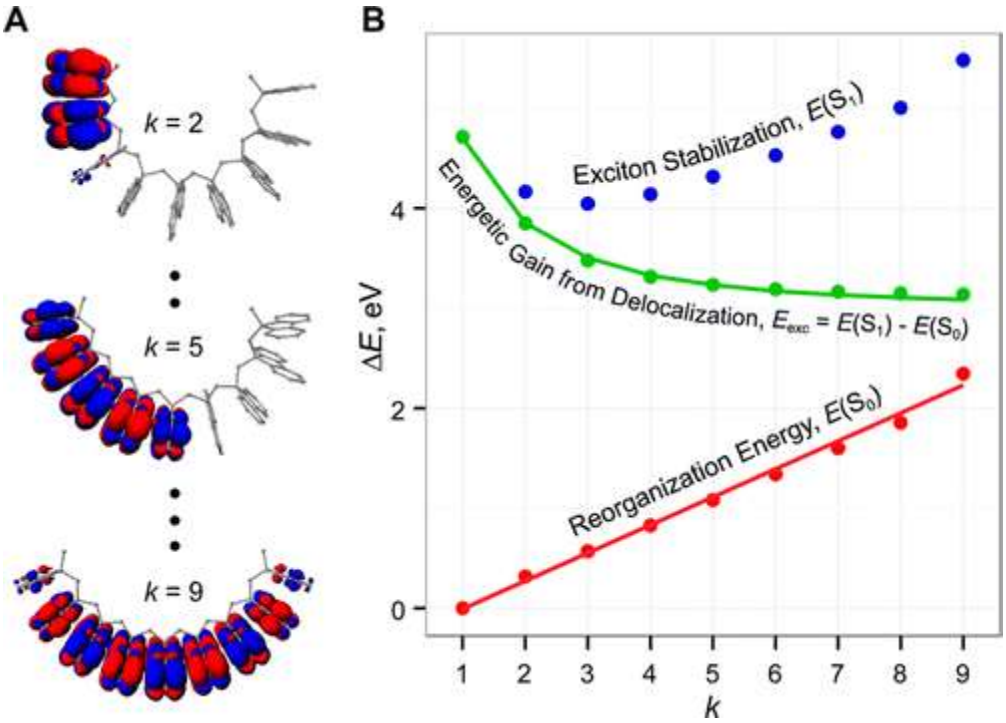

Figure 5. Transition density plots corresponding to the $S_0 \rightarrow S_1$ vertical excitation (A) and energies of the S_0 and S_1 states and the corresponding $E_{exc} = E(S_1) - E(S_0)$ (B) in F9 with a different number (k) of eclipsed fluorene units (see the section S7 in the SI for details). Note that data points for $E(S_0)$ and E_{exc} were fitted by the linear and $\cos \pi/(k + 1)$ trends, respectively.

The energies of the structures $E(S_0)$ increased linearly with increasing k, suggesting that the reorganization penalty increases linearly with addition of each fluorene in an eclipsed sandwich-like arrangement, Figure 5B. On the other hand, the excitation energies (E_{exc}), evaluated from the difference of the ground- [$E(S_0)$] and excited- [$E(S_1)$] state energies of various F9 structures, saturate with an increasing number of sandwiched fluorenes (k), and the evolution of $E_{exc}(k)$ follows a familiar $\cos \pi/(k + 1)$ trend (Figure 5B).[30-33] Thus, the extent of exciton delocalization should be governed by a cumulative effect of the quickly saturating energetic gain from exciton delocalization and the linearly increasing energetic penalty for conformational reorganization. Due to this interplay, the most effective stabilization of the exciton, that is, the lowest $E(S_1)$, is achieved when the exciton is confined on a limited number of chromophores, for example, three units in the model structure F9 as judged by the presence of a minimum on the $E(S_1)$ curve in Figure 5B. (Note that the

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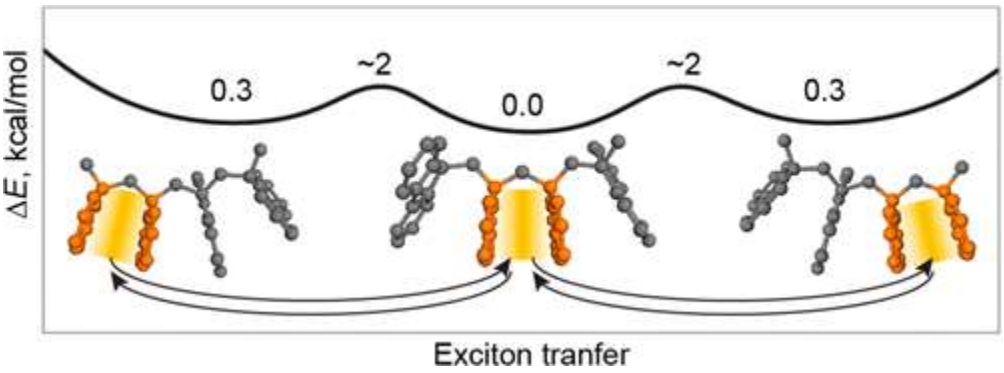
bond length changes within fluorenes lead to further localization of the exciton to only two units, vide supra.)

The localization of the exciton onto only two units raises the question of the mechanism and efficiency of exciton transfer along the multichromophoric assembly. To examine this issue, we return to F4, which is the smallest assembly that shows two distinct valence tautomers that are nearly isoenergetic with an energy difference of only 0.3 kcal/mol (Scheme 1). The transition state of the exciton transfer or interconversion between these valence tautomers is expected to involve a structure in which the exciton is delocalized on three fluorenes arranged in a sandwich-like configuration. The energetic cost of the formation of F3 in its fully eclipsed conformation is ~2 kcal/mol, and thus, a similar energetic expenditure is expected for the transition state of the F4 tautomer interconversion. Therefore, the coexistence of such tautomers and a low (~2 kcal/mol) barrier of their interconversion indicates a possible mechanism of exciton transfer that involves hopping along the multichromophoric π-stacked assembly (Scheme 1). The nonadiabatic exciton transfer in Scheme 1 via coupling with the associated torsional mode (Figure S4 in the SI) is unlikely as this torsional mode is of extremely low frequency (in the 13–17 cm^{-1} range, Table S19 in the SI), unlike the linearly connected π-conjugated systems where the normal modes associated with the exciton transfer are generally of high frequency.[34]



Scheme 1. Potential Energy Profile of the Singlet Exciton Transfer along the Covalently Linked π-Array of Fluorene Chromophores on the Representative Example of F4

In summary, we undertook a computational study of cofacially arrayed π-stacked polyfluorenes in their ground (S_0) and first excited (S_1) states by means of the TD-DFT calculations based on the carefully

calibrated B1LYP-40 density functional. The calculations successfully reproduced the spectroscopic observation of the excimeric state (i.e., exciton delocalization to only two fluorene units) in F2 as well as larger polyfluorenes. In such an excimeric state, excitation-induced bond length changes were evenly distributed over both fluorene units and were half of those observed in monomeric F1. Using a model structure, F9, we demonstrated that the extent of the exciton delocalization (e.g., two units in cofacially arrayed polyfluorenes) is shaped by the interplay between the quickly saturating energetic gain from the delocalization and the linearly increasing reorganization penalty due to the requirement for the perfectly eclipsed sandwich-like arrangement of all involved fluorenes. Localization of the exciton onto two units in F4 and higher polyfluorenes allows for the existence of nearly isoenergetic (within 0.3 kcal/mol) valence tautomers, which differ in the position of the exciton in the polyfluorene chain. The presence of such tautomers and the plausibility of their ready interconversion over a modest (~2 kcal/mol) activation barrier suggests that exciton hopping is a plausible mechanism of singlet energy transfer along the multichromophoric π-stacked assembly in polyfluorenes.

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[26]$F2^{S1}$ has only one electronic structure, while $F3^{S1}$ can exist in two indistinguishable mirror-image valence tautomers. On the other hand,

large F*n* will have two *n*/2 and (*n* – 1)/2 distinct structures for even and odd *n*, respectively.

[27]Because two fluorene units are arranged in a completely eclipsed manner, the transition dipole moments for the lowest excited state (S_1) are antiparallel, which would lead to a forbidden $S_1 \rightarrow S_0$ transition, that is, the oscillator strength is expected to be zero. However, a slight misorientation due to torsional vibrations in the excited state gives rise to a discernable oscillator strength and as such also accounts for the long lifetimes of excimers. Also, see Table S18 in the SI for additional details and Diri, K.; Krylov, A. I.Electronic States of the Benzene Dimer: A Simple Case of Complexity *J. Phys. Chem. A* 2012, 116, 653– 662, DOI: 10.1021/jp209190e

[28]Note that the additional reorganization penalty of 3.9 kcal/mol in $F3'^{S1}$ is somewhat lower than the conformational reorganization penalty of 5.6 kcal/mol in $F2^{S1}$, most likely due to the choice of fixed geometrical parameters in the constrained optimization of $F3'^{S1}$.

[29]It is noted that similar attempts to obtain the exciton delocalized onto four units in F4 by imposing the eclipsed π-stacked arrangement of all fluorenes were unsuccessful and led to a structure in which the exciton was localized onto two units. Such a localization of exciton is likely related to the energetic penalty from the bond length changes within fluorenes and is somewhat similar to the localization of the polaron in mixed-valence systems due to the interplay of electronic coupling and reorganization energy; see e.g.: Brunschwig, B. S.; Creutz, C.; Sutin, N.Optical transitions of symmetrical mixed-valence systems in the Class II–III transition regime *Chem. Soc. Rev.* 2002, 31, 168, DOI: 10.1039/b008034i

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Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jpclett.6b01268.

- Materials and methods, figures showing optical spectra, homodesmic analysis, transition density plots, the visual representation of the torsional modes, and tables showing energetics, bond lengths, oscillator strengths, frequencies of the torsional modes, as well as the Python script for the structure of F9 and an archive of the calculation files (PDF)

Supporting Information

Two's Company, Three's a Crowd: Exciton Localization in Cofacially-Arrayed Polyfluorenes

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Table of contents:

S1. The Generation and Optical Spectroscopy of $F1^{+\bullet}$-$F6^{+\bullet}$

The **F2-F6** cation radicals were generated using either a hindered naphthalene (i.e. 1,2,3,4,7,8,9,10-octahydro-1,1,4,4,7,7,10,10-octamethylnaphtacene) cation radical (E_{red} = 0.94 V vs Fc/Fc^+, λ_{max} = 672 nm, ε_{max} = 9300 $cm^{-1}M^{-1}$) or NO^+ $SbCl_6^-$ as oxidants[1] in anhydrous dichloromethane in the presence of excess **F2**-**F6** at ambient temperature. The UV-vis-NIR absorption spectra of the resulting colored solutions were recorded and compiled in Figure S1. Note that the **F2** cation radical was somewhat unstable and decomposed within minutes. Also note that owing to the high oxidation potential of parent 9,9-dimethylfluorene (**F1**), its cation radical was generated using transient laser-flash photolysis technique,[1] where a diffusional electron-transfer quenching of the photoexcited chloranil triplet as an oxidant (E_{red} = 2.2 V vs SCE) with **F1** produced its characteristic cation radical spectrum (Figure S1).

A comparison of the absorption spectra of **F2-F6** cation radicals with that of the transient **F1** cation radical showed that the cation radical derived from cofacially-stacked polyfluorenes **F2-F6** had intense charge-resonance absorptions in the near infrared (NIR) region which shifts red with increasing number of fluorene moieties in **F2-F6**. The presence of NIR transitions in polyfluorenes is highly indicative of the hole hopping through stacked π-systems.[2]

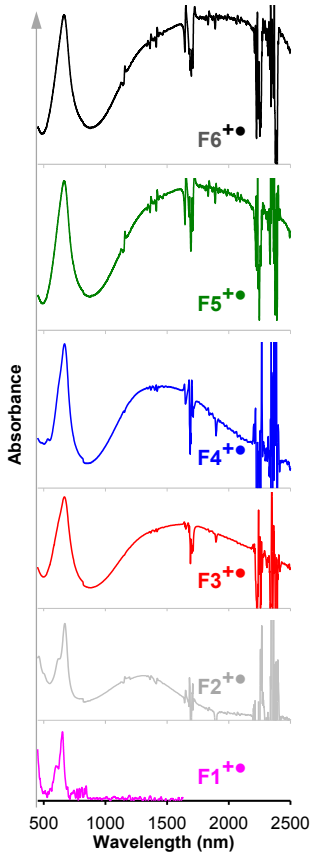


Figure S1. Optical spectra of $F1^{+\bullet}$-$F6^{+\bullet}$ generated using $NO^+SbCl_6^-$ in CH_2Cl_2 at 22 °C. Note that $F1^{+\bullet}$ was generated via laser-flash photolysis.

S2. Computational Details

Electronic structure calculations were performed with the Gaussian 09 package, revision D01.[3] For the density functional theory (DFT) calculations we used calibrated (see Ref. [4] for details, also see refs [5-9])

B1LYP functional[10] that contains 40% contribution of the exact exchange with 6-31G(d) basis set by Pople and co-workers.[11] For comparison, we also used standard functional ωB97X-D in combination with the 6-31G(d) basis set as well as PBE0 density functional[12,13] augmented with D3 version of Grimme's dispersion term[14] in combination with the double-ζ def2-SV(P) basis by Weigend and Ahlrichs.[15] Solvent effects were included using the implicit integral equation formalism polarizable continuum model (IEF-PCM, also referred as PCM)[16-20] with the dichloromethane solvent parameters (ε = 8.93). In all DFT calculations, ultrafine Lebedev's grid was used with 99 radial shells per atom and 590 angular points in each shell. Energy calculations and geometry optimizations performing using the time-dependent density functional theory (TD-DFT) method.[21-27] Tight cutoffs on forces and atomic displacement were used to determine convergence in geometry optimization procedure. Hessians were calculated for the optimized structures of **F1**-**F6** in the ground electronic state and **F1**-**F3** in the excited (S_1) state to confirm absence of imaginary frequencies.

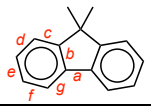
S3. Energetics of the Excitation/Emission Cycles of F1-F6

Table S1. Energetics (in kcal/mol) of the excitation/emission cycles of **F1**-**F6**. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Effects of the solvent in the excited state were accounted via the state-specific approach. The target state in absorption/emission was calculated with non-equilibrium solvation based on the information from the initial state.

Fn	Level of Theory	E_{abs}	λ_1	E_{em}	λ_0
F1	B1LYP-40/6-31G(d)	112.82	7.00	97.10	8.71
	PBE0-D3/def2-SV(P)	108.11	4.90	96.16	7.05
	ωB97X-D/6-31G(d)	114.26	6.85	98.22	9.19
F2	B1LYP-40/6-31G(d)	109.77	15.29	79.88	14.61
	PBE0-D3/def2-SV(P)	91.64	8.98	67.62	15.03
	ωB97X-D/6-31G(d)	110.57	16.54	78.77	15.26
F3	B1LYP-40/6-31G(d)	108.95	15.68	78.76	14.52
	PBE0-D3/def2-SV(P)	88.24	7.91	64.95	15.38
	ωB97X-D/6-31G(d)	109.21	16.05	77.34	15.82
F4	B1LYP-40/6-31G(d)	108.40	15.63	78.26	14.51
	PBE0-D3/def2-SV(P)	87.30	8.06	63.53	15.72
	ωB97X-D/6-31G(d)	108.79	15.82	76.96	16.01
F5	B1LYP-40/6-31G(d)	107.96	15.73	78.17	14.06
	PBE0-D3/def2-SV(P)	87.28	5.80	65.76	15.71
	ωB97X-D/6-31G(d)	108.73	15.45	76.96	16.32
F6	B1LYP-40/6-31G(d)	107.80	15.80	77.76	14.24
	PBE0-D3/def2-SV(P)	86.82	5.54	65.58	15.69
	ωB97X-D/6-31G(d)	108.60	15.63	76.65	16.32

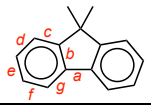
S4. Structural Parameters of F1-F6

Table S2. Aromatic carbon-carbon bond lengths (in Å, indicated in the structure) of **F1**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.



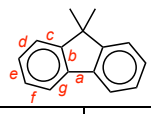
	B1LYP-40/6-31G(d)	PBE0-D3/def2-SV(P)	ωB97X-D/6-31G(d)
	F	F	F
a	1.467	1.465	1.470
b	1.402	1.407	1.402
c	1.385	1.390	1.387
d	1.394	1.399	1.396
e	1.393	1.399	1.396
f	1.391	1.396	1.394
g	1.390	1.396	1.392

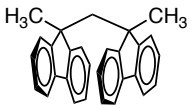
Table S3. Aromatic carbon-carbon bond lengths (in Å, indicated in the structure) of **F1**^{S1}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



	B1LYP-40/6-31G(d)	PBE0-D3/def2-SV(P)	ωB97X-D/6-31G(d)
	F	F	F
a	1.387	1.396	1.386
b	1.457	1.456	1.459
c	1.368	1.375	1.371
d	1.411	1.418	1.413
e	1.417	1.420	1.419
f	1.369	1.378	1.373
g	1.440	1.442	1.443

Table S4. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F2**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.

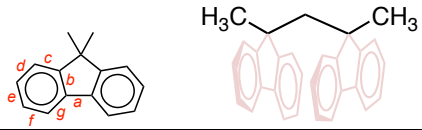




	B1LYP-40/6-31G(d)		PBE0-D3/def2-SV(P)		ωB97X-D/6-31G(d)	
	F	F	F	F	F	F
a	1.465	1.465	1.464	1.464	1.469	1.468
b	1.400	1.402	1.406	1.407	1.401	1.401

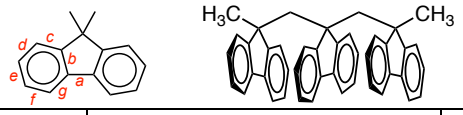
c	1.385	1.386	1.389	1.39	1.386	1.387
d	1.394	1.393	1.399	1.397	1.396	1.394
e	1.393	1.393	1.399	1.400	1.396	1.396
f	1.391	1.390	1.396	1.395	1.394	1.393
g	1.390	1.391	1.395	1.396	1.390	1.391

Table S5. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F2**^{S1}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



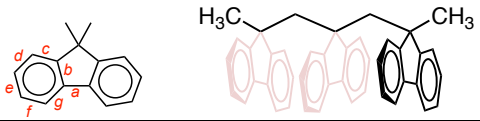
	B1LYP-40/6-31G(d)		PBE0-D3/def2-SV(P)		ωB97X-D/6-31G(d)	
	F	F	F	F	F	F
a	1.420	1.420	1.424	1.424	1.422	1.422
b	1.429	1.429	1.431	1.431	1.429	1.428
c	1.376	1.377	1.380	1.380	1.377	1.377
d	1.399	1.399	1.407	1.407	1.402	1.402
e	1.409	1.409	1.411	1.411	1.409	1.409
f	1.377	1.377	1.384	1.383	1.380	1.380
g	1.416	1.416	1.419	1.419	1.417	1.417

Table S6. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F3**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.



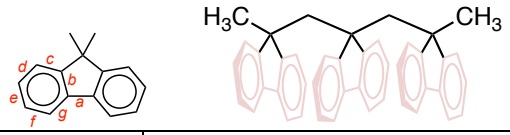
	B1LYP-40/6-31G(d)			PBE0-D3/def2-SV(P)			ωB97X-D/6-31G(d)		
	F	F	F	F	F	F	F	F	F
a	1.465	1.464	1.465	1.463	1.463	1.463	1.468	1.467	1.468
b	1.400	1.403	1.4	1.405	1.406	1.405	1.400	1.400	1.400
c	1.385	1.385	1.385	1.389	1.390	1.390	1.386	1.387	1.386
d	1.394	1.392	1.394	1.399	1.395	1.399	1.396	1.391	1.396
e	1.393	1.393	1.393	1.399	1.400	1.399	1.395	1.396	1.395
f	1.391	1.390	1.391	1.396	1.394	1.396	1.394	1.392	1.394
g	1.390	1.390	1.39	1.395	1.396	1.395	1.39	1.391	1.390

Table S7. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F3**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



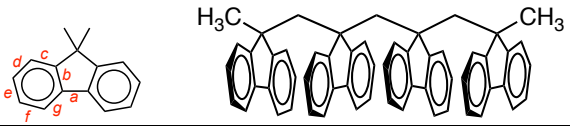
	B1LYP-40/6-31G(d)			PBE0-D3/def2-SV(P)			ωB97X-D/6-31G(d)		
	F	F	F	F	F	F	F	F	F
a	1.421	1.418	1.465	1.424	1.423	1.463	1.421	1.42	1.468
b	1.428	1.43	1.4	1.431	1.431	1.405	1.429	1.428	1.400
c	1.375	1.376	1.385	1.379	1.379	1.390	1.377	1.376	1.387
d	1.400	1.399	1.394	1.408	1.403	1.399	1.402	1.398	1.396
e	1.408	1.408	1.393	1.411	1.412	1.399	1.409	1.409	1.396
f	1.377	1.376	1.391	1.384	1.382	1.396	1.38	1.379	1.394
g	1.415	1.415	1.390	1.419	1.418	1.394	1.417	1.415	1.390

Table S8. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F3'**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.



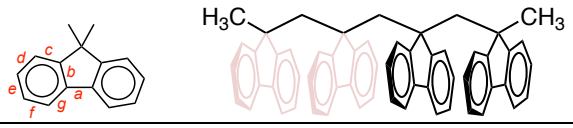
	B1LYP-40/6-31G(d)			PBE0-D3/def2-SV(P)			ωB97X-D/6-31G(d)		
	F	F	F	F	F	F	F	F	F
a	1.449	1.411	1.443	1.447	1.421	1.442	1.457	1.411	1.443
b	1.410	1.434	1.413	1.417	1.430	1.418	1.408	1.433	1.414
c	1.383	1.376	1.382	1.385	1.379	1.384	1.384	1.374	1.381
d	1.393	1.396	1.394	1.402	1.404	1.403	1.396	1.400	1.398
e	1.400	1.413	1.402	1.404	1.412	1.405	1.399	1.412	1.403
f	1.385	1.373	1.383	1.391	1.382	1.389	1.389	1.376	1.386
g	1.399	1.420	1.402	1.406	1.418	1.408	1.397	1.421	1.404

Table S9. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F4**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.



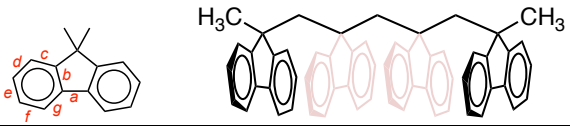
	B1LYP-40/6-31G(d)			
	F	F	F	F
a	1.465	1.464	1.464	1.465
b	1.402	1.398	1.403	1.4
c	1.386	1.385	1.385	1.385
d	1.393	1.394	1.392	1.394
e	1.393	1.393	1.393	1.393
f	1.39	1.391	1.39	1.391
g	1.391	1.389	1.39	1.39
	PBE0-D3/def2-SV(P)			
	F	F	F	F
a	1.463	1.462	1.462	1.463
b	1.407	1.404	1.406	1.405
c	1.39	1.389	1.39	1.39
d	1.397	1.398	1.395	1.399
e	1.4	1.398	1.4	1.399
f	1.395	1.396	1.394	1.396
g	1.396	1.394	1.396	1.395
	ωB97X-D/6-31G(d)			
	F	F	F	F
a	1.468	1.466	1.467	1.468
b	1.401	1.399	1.4	1.4
c	1.387	1.385	1.386	1.386
d	1.394	1.395	1.391	1.396
e	1.396	1.395	1.396	1.396
f	1.393	1.394	1.392	1.394
g	1.392	1.389	1.391	1.39

Table S10. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F4**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



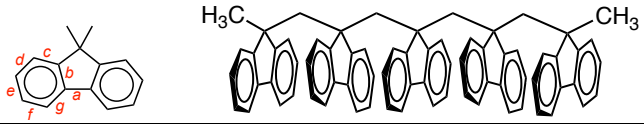
		B1LYP-40/6-31G(d)		
	F	F	F	F
a	1.421	1.418	1.463	1.465
b	1.428	1.427	1.403	1.400
c	1.376	1.377	1.385	1.385
d	1.400	1.399	1.393	1.394
e	1.408	1.409	1.393	1.393
f	1.377	1.376	1.390	1.391
g	1.416	1.416	1.390	1.390
		PBE0-D3/def2-SV(P)		
	F	F	F	F
a	1.425	1.422	1.461	1.464
b	1.431	1.428	1.406	1.405
c	1.380	1.380	1.390	1.389
d	1.408	1.405	1.396	1.399
e	1.410	1.411	1.399	1.399
f	1.385	1.382	1.394	1.396
g	1.419	1.417	1.396	1.395
		ωB97X-D/6-31G(d)		
	F	F	F	F
a	1.421	1.420	1.466	1.468
b	1.429	1.426	1.400	1.400
c	1.377	1.377	1.386	1.386
d	1.402	1.400	1.392	1.396
e	1.409	1.409	1.396	1.395
f	1.380	1.379	1.392	1.394
g	1.417	1.415	1.391	1.390

Table S11. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F4'**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



		B1LYP-40/6-31G(d)		
	F	F	F	F
a	1.465	1.419	1.419	1.464
b	1.403	1.426	1.430	1.400
c	1.386	1.375	1.375	1.385
d	1.393	1.400	1.400	1.394
e	1.393	1.408	1.408	1.393
f	1.390	1.376	1.376	1.391
g	1.391	1.416	1.415	1.390
		PBE0-D3/def2-SV(P)		
	F	F	F	F
a	1.463	1.422	1.422	1.463
b	1.407	1.428	1.431	1.405
c	1.390	1.379	1.379	1.390
d	1.398	1.406	1.405	1.399
e	1.399	1.411	1.411	1.399
f	1.395	1.383	1.383	1.397
g	1.396	1.418	1.418	1.395
		ωB97X-D/6-31G(d)		
	F	F	F	F
a	1.468	1.419	1.419	1.467
b	1.402	1.425	1.428	1.400
c	1.387	1.376	1.376	1.387
d	1.394	1.401	1.399	1.396
e	1.396	1.409	1.409	1.396
f	1.393	1.379	1.379	1.394
g	1.392	1.416	1.416	1.390

Table S12. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F5**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.

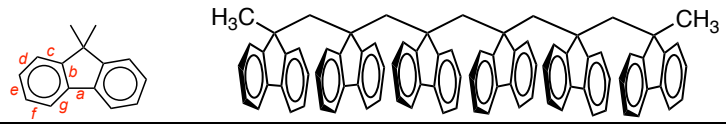


			B1LYP-40/6-31G(d)		
	F	F	F	F	F
a	1.465	1.464	1.463	1.464	1.465
b	1.402	1.398	1.398	1.403	1.400
c	1.386	1.385	1.385	1.385	1.385
d	1.393	1.393	1.393	1.392	1.394
e	1.393	1.393	1.393	1.393	1.393
f	1.390	1.391	1.391	1.390	1.391
g	1.391	1.389	1.389	1.390	1.390
			PBE0-D3/def2-SV(P)		
	F	F	F	F	F
a	1.464	1.462	1.462	1.462	1.464
b	1.407	1.404	1.404	1.406	1.405
c	1.39	1.389	1.389	1.39	1.39
d	1.397	1.398	1.398	1.395	1.399
e	1.400	1.398	1.398	1.400	1.399
f	1.395	1.396	1.396	1.394	1.396
g	1.396	1.394	1.393	1.396	1.395
			ωB97X-D/6-31G(d)		
	F	F	F	F	F
a	1.468	1.466	1.466	1.466	1.468
b	1.401	1.399	1.398	1.400	1.400
c	1.387	1.385	1.385	1.386	1.386
d	1.394	1.395	1.395	1.391	1.396
e	1.396	1.395	1.395	1.396	1.396
f	1.393	1.394	1.394	1.392	1.394
g	1.391	1.389	1.389	1.391	1.390

Table S13. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F5**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.

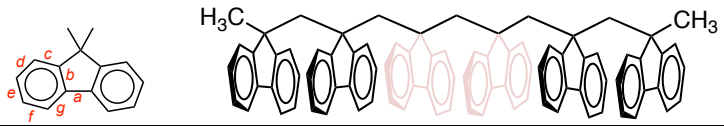
			B1LYP-40/6-31G(d)		
	F	F	F	F	F
a	1.465	1.419	1.418	1.463	1.465
b	1.403	1.426	1.426	1.403	1.400
c	1.386	1.375	1.375	1.385	1.385
d	1.393	1.400	1.400	1.393	1.394
e	1.393	1.408	1.408	1.393	1.393
f	1.390	1.377	1.376	1.390	1.391
g	1.391	1.416	1.416	1.390	1.390
			PBE0-D3/def2-SV(P)		
	F	F	F	F	F
a	1.463	1.423	1.422	1.461	1.464
b	1.407	1.428	1.428	1.406	1.405
c	1.390	1.379	1.379	1.390	1.389
d	1.398	1.406	1.406	1.396	1.399
e	1.399	1.411	1.411	1.399	1.399
f	1.395	1.383	1.383	1.394	1.396
g	1.396	1.418	1.418	1.396	1.395
			ωB97X-D/6-31G(d)		
	F	F	F	F	F
a	1.468	1.420	1.419	1.466	1.468
b	1.402	1.425	1.425	1.401	1.400
c	1.387	1.376	1.376	1.386	1.386
d	1.394	1.401	1.401	1.392	1.396
e	1.396	1.409	1.409	1.396	1.395
f	1.393	1.379	1.379	1.392	1.394
g	1.392	1.416	1.416	1.391	1.390

Table S14. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F6**^{S0}. The PCM(CH_2Cl_2) solvation model was utilized in all calculations.



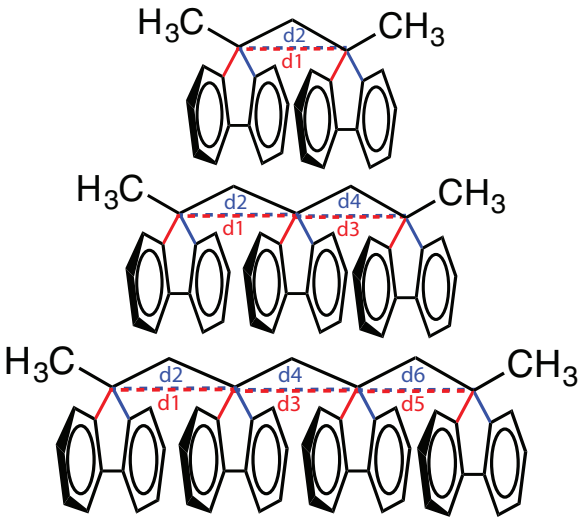
			B1LYP-40/6-31G(d)			
	F	F	F	F	F	F
a	1.465	1.464	1.464	1.463	1.464	1.465
b	1.402	1.403	1.398	1.398	1.403	1.400
c	1.386	1.385	1.385	1.385	1.385	1.385
d	1.393	1.392	1.393	1.393	1.392	1.394
e	1.393	1.393	1.393	1.393	1.393	1.393
f	1.390	1.390	1.391	1.391	1.390	1.391
g	1.391	1.390	1.389	1.389	1.390	1.39
			PBE0-D3/def2-SV(P)			
	F	F	F	F	F	F
a	1.463	1.462	1.462	1.462	1.462	1.463
b	1.407	1.406	1.404	1.404	1.406	1.405
c	1.390	1.390	1.389	1.389	1.390	1.390
d	1.397	1.395	1.398	1.398	1.395	1.399
e	1.400	1.400	1.398	1.398	1.400	1.399
f	1.395	1.394	1.396	1.396	1.394	1.396
g	1.396	1.396	1.393	1.393	1.396	1.395
			ωB97X-D/6-31G(d)			
	F	F	F	F	F	F
a	1.468	1.466	1.466	1.466	1.466	1.468
b	1.401	1.400	1.398	1.398	1.400	1.400
c	1.387	1.387	1.385	1.385	1.386	1.386
d	1.394	1.391	1.395	1.395	1.391	1.396
e	1.396	1.396	1.395	1.395	1.396	1.396
f	1.393	1.392	1.394	1.394	1.392	1.394
g	1.391	1.391	1.389	1.389	1.391	1.390

Table S15. Aromatic carbon-carbon bond lengths (in Å, indicated in the left structure) within fluorenes (one column for each fluorene moiety) of **F6**[S1]. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



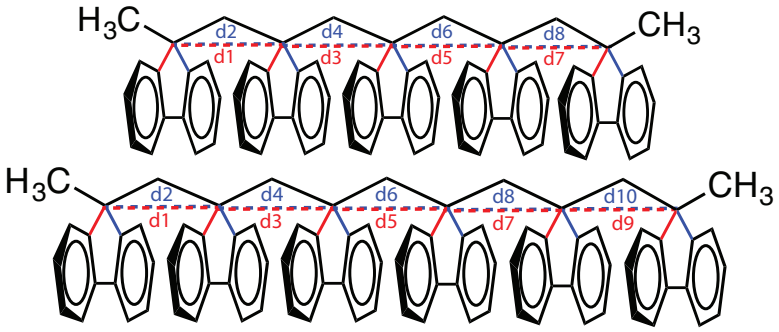
			B1LYP-40/6-31G(d)			
	F	F	F	F	F	F
a	1.465	1.463	1.418	1.419	1.463	1.465
b	1.402	1.403	1.425	1.425	1.403	1.400
c	1.386	1.385	1.375	1.375	1.385	1.385
d	1.393	1.393	1.401	1.400	1.393	1.394
e	1.393	1.393	1.408	1.408	1.393	1.393
f	1.390	1.390	1.376	1.376	1.390	1.391
g	1.391	1.390	1.416	1.416	1.390	1.390
			PBE0-D3/def2-SV(P)			
	F	F	F	F	F	F
a	1.464	1.461	1.422	1.422	1.461	1.464
b	1.407	1.407	1.427	1.427	1.407	1.405
c	1.390	1.390	1.379	1.379	1.390	1.389
d	1.397	1.396	1.407	1.407	1.396	1.399
e	1.400	1.399	1.411	1.410	1.399	1.399
f	1.395	1.394	1.383	1.383	1.394	1.396
g	1.396	1.396	1.418	1.418	1.396	1.395
			ωB97X-D/6-31G(d)			
	F	F	F	F	F	F
a	1.468	1.466	1.419	1.419	1.465	1.468
b	1.401	1.400	1.425	1.425	1.401	1.400
c	1.387	1.386	1.376	1.376	1.387	1.386
d	1.394	1.392	1.401	1.401	1.392	1.396
e	1.396	1.396	1.409	1.409	1.396	1.395
f	1.393	1.392	1.379	1.379	1.392	1.394
g	1.392	1.391	1.416	1.416	1.391	1.390

Table S16. Dihedral angles (in degrees) between adjacent fluorene units in **F1^{S0}-F4^{S0}** and **F1^{S1}-F4^{S1}** series. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



	S0			S1		
	B1LYP-40	PBE0-D3	ωB97X-D	B1LYP-40	PBE0-D3	ωB97X-D
		F2			**F2**	
d1	-26.9	-25.4	-24.9	0.3	0.2	0.2
d2	-26.9	-25.4	-24.9	0.3	0.3	0.2
		F3			**F3**	
d1	28.5	25.6	25.2	0.0	-0.2	-0.1
d2	27.1	25.1	24.8	-0.7	-0.4	-0.3
d3	-28.0	-25.4	-25.0	-34.2	-28.6	-28.3
d4	-29.4	-25.9	-25.4	-35.2	-29.0	-28.7
		F4			**F4**	
d1	-27.7	-25.8	-25.6	-25.3	-25.3	-25.1
d2	-26.0	-25.2	-25.0	-23.7	-24.7	-24.5
d3	30.1	26.0	25.5	38.9	34.6	29.2
d4	30.1	26.0	25.5	38.4	34.4	29.2
d5	-25.6	-25.1	-24.9	0.8	0.5	0.7
d6	-27.3	-25.8	-25.5	0.0	0.2	0.5
		F4			**F4'**	
d1	-27.7	-25.8	-25.6	34.8	32.8	32.3
d2	-26.0	-25.2	-25.0	35.9	33.1	32.7
d3	30.1	26.0	25.5	0.6	0.7	0.8
d4	30.1	26.0	25.5	0.6	0.7	0.8
d5	-25.6	-25.1	-24.9	37.2	33.3	32.1
d6	-27.3	-25.8	-25.5	36.1	32.9	31.7

Table S17. Dihedral angles (in degrees) between adjacent fluorene units in **F5^{S0}-F6^{S0}** and **F5^{S1}-F6^{S1}** series. The PCM(CH_2Cl_2) solvation model was utilized in all calculations. Highlighted units represent exciton localization.



	S0			S1		
	B1LYP-40	PBE0-D3	ωB97X-D	B1LYP-40	PBE0-D3	ωB97X-D
	F5			**F5**		
d1	26.0	24.9	24.6	34.9	32.9	32.3
d2	27.7	25.5	25.2	36.0	33.2	32.8
d3	-26.7	-26.1	-25.9	0.7	1.0	1.1
d4	-26.4	-26.0	-25.8	0.8	1.1	1.1
d5	30.5	26.7	26.5	37.9	33.8	33.0
d6	30.2	26.6	26.3	38.2	34.0	33.2
d7	-28.1	-26.4	-26.2	-27.2	-25.1	-24.6
d8	-26.4	-25.7	-25.5	-25.6	-24.4	-23.9
	F6			**F6**		
d1	-26.9	-25.7	-25.6	-23.9	-24.5	-23.5
d2	-28.6	-26.3	-26.2	-25.6	-25.2	-24.1
d3	29.3	26.9	26.3	39.1	37.8	35.0
d4	29.0	26.8	26.2	39.4	38.1	35.2
d5	-25.6	-25.8	-25.7	1.0	1.2	1.7
d6	-25.5	-25.8	-25.7	1.0	1.1	1.7
d7	31.3	27.0	26.1	38.4	36.7	36.9
d8	31.6	27.1	26.2	38.1	36.4	36.7
d9	-27.3	-26.5	-26.1	-25.0	-24.8	-24.0
d10	-25.6	-25.8	-25.4	-23.4	-24.1	-23.4

S5. Analysis of F1 Electron Densities in Different Electronic States Using a Frozen Orbital Approximation

Observation that the excitation-induced bond length changes in **F1** correspond to the sum of the oxidation- and reduction-induced bond length changes (i.e. $\Delta R^{S1} \approx \Delta R^{+\bullet} + \Delta R^{-\bullet}$) can be easily reconciled based on the fact that formation of the excited state involves promotion of an electron from HOMO to LUMO. Thus, molecular electron density can be expressed in the basis of canonical molecular orbitals at any point in space $\vec{x}$ as:

$$\rho(\vec{x}) = \sum_{i=1}^{n} \chi_i^2(\vec{x}) \qquad \text{(S1)}$$

where $\chi_i(\vec{x})$ are the molecular orbitals (considered as real functions), and *n* is size of the basis set. By making the assumption that orbitals of the excited state are identical to those of the ground state (frozen orbital approximation), it directly follows from eq S1 that:

$$\Delta\rho^{S1}(\vec{x}) = \rho^{S1}(\vec{x}) - \rho^{N}(\vec{x}) = \chi^2_{\mathrm{LUMO}}(\vec{x}) - \chi^2_{\mathrm{HOMO}}(\vec{x}) \qquad \text{(S2)}$$

where χ_{HOMO} and χ_{LUMO} are the molecular HOMO and LUMO, respectively. Furthermore, the terms $\chi^2_{\mathrm{HOMO}}(\vec{x})$ and $\chi^2_{\mathrm{LUMO}}(\vec{x})$ can be expressed by using eq S1 and frozen orbital approximation via the cation- and anion-radical electron densities of a molecule:

$$\chi^2_{\mathrm{HOMO}}(\vec{x}) = \rho^{N}(\vec{x}) - \rho^{CR}(\vec{x}) = -\Delta\rho^{CR}(\vec{x}) \qquad \text{(S3a)}$$
$$\chi^2_{\mathrm{LUMO}}(\vec{x}) = \rho^{AR}(\vec{x}) - \rho^{N}(\vec{x}) = \Delta\rho^{AR}(\vec{x}) \qquad \text{(S3b)}$$

Therefore, the difference in the electron densities of the ground and excited states ($\Delta\rho^{S1}$) can be expressed using eqs S2 and S3 as:

$$\Delta\rho^{S1}(\vec{x}) = \Delta\rho^{AR}(\vec{x}) + \Delta\rho^{CR}(\vec{x}) \qquad \text{(S4)}$$

which is consistent with the observed bond length changes in the excited, cation- and anion-radical states of **F1** (i.e. $\Delta R^{S1} \approx \Delta R^{+\bullet} + \Delta R^{-\bullet}$).

Usage of the frozen orbital approximation is validated by the comparison of atomic charges of **F1** in neutral, S1, cation- and anion-radical states and observation that:

$$\Delta q^{S1} \sim \Delta q^{+\bullet} + \Delta q^{-\bullet}$$

where charges were calculated at the equilibrium geometries of the corresponding electronic states. Note that due to the close spatial overlay of HOMO and LUMO, the $\Delta q^{+\bullet}$ and $\Delta q^{-\bullet}$ terms mostly cancel out each other, and therefore the atomic charges in **F1**^{S1} are quite similar to those in the ground state.

S6. Homodesmic Analysis of Reorganization Penalty in F2

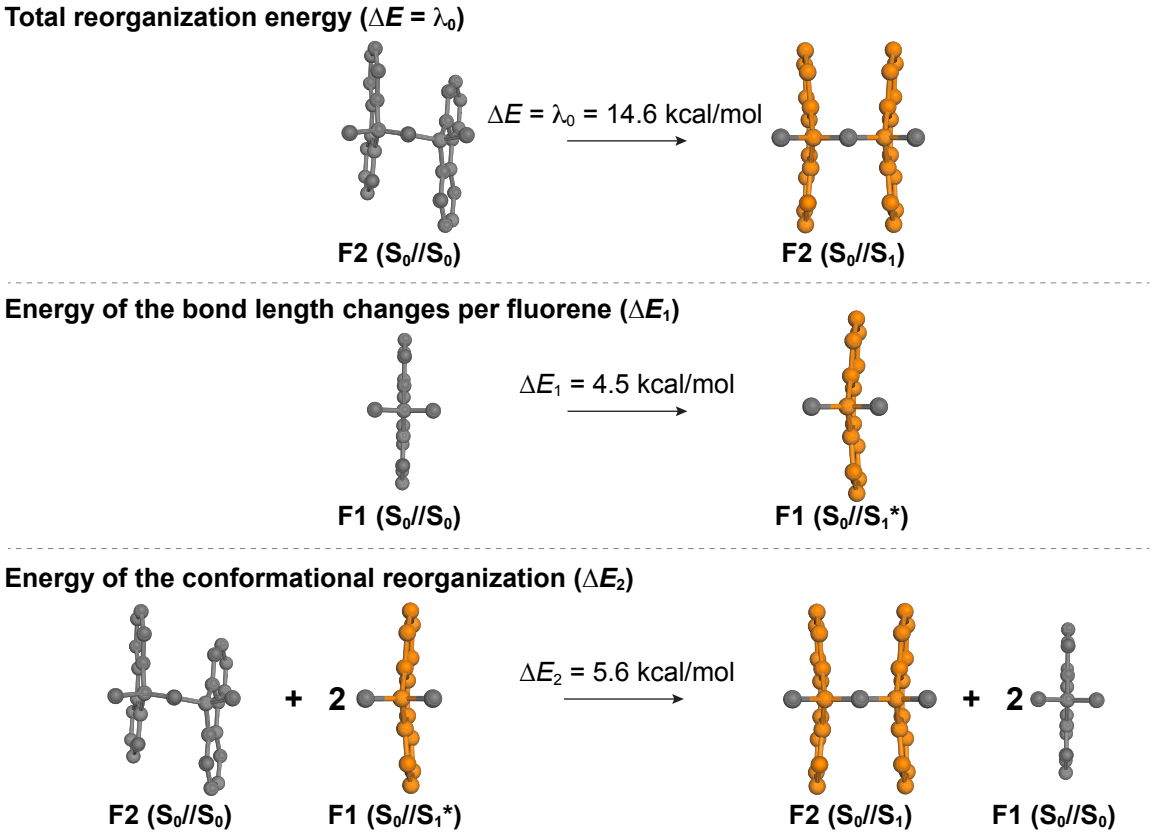


Figure S2. Homodesmic analysis of the reorganization penalty [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)]. The double-slash notation indicates the electronic state (first value) and geometry (second value) at which the calculation of energy was performed. The **F1** (S0//S1*) notation indicates that electronic energy of **F1** was evaluated at the geometry that corresponds to the geometry of a fluorene moiety in **F2**[S1].

S7. Oscillator Strength of F2

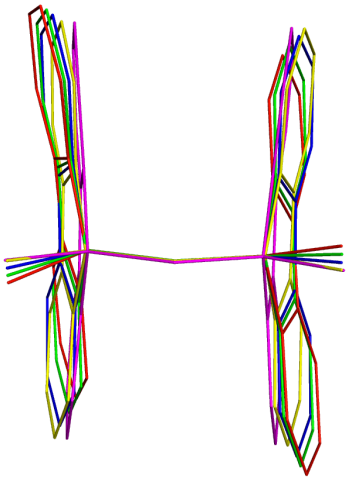
The strength of an electronic transition depends on the transition dipole moment between two states. For two noninteracting molecules, the transition dipole moments are $\vec{\mu}_1 = \langle \psi_1 | e\vec{r} | \psi_1^* \rangle$ and $\vec{\mu}_2 = \langle \psi_2 | e\vec{r} | \psi_2^* \rangle$. Then, the transition moment for the two states of two electronically coupled molecules is given by

$$\vec{\mu}_{\mp} = \frac{1}{\sqrt{2}} \left(\vec{\mu}_1 \mp \vec{\mu}_2 \right)$$

Thus, the transition dipole moment depends on the relative orientation of the two molecules. In case when the two molecules are arranged in an eclipsed manner (H-type interaction), the transition dipole can be arranged in parallel or anti-parallel fashion. In antiparallel arrangement two dipole moments add up to a value of zero and correspond to a forbidden transition, while in the parallel arrangement the dipole moment is enhanced to a value of $2\vec{\mu}_1$, which corresponds to the allowed transition. However, in reality a slight misorientation due to the molecular vibrations gives rise to a weak transition dipole moment, so that a long-lived emission is observed.

Since localization of the exciton in the **Fn** series requires an eclipsed configuration of two fluorene units, the total transition dipole moment between ground S_0 and lowest excited state (S_1) adds up to a value of zero, leading to zero value of oscillator strength and a forbidden S_1->S_0 transition. To verify that the geometrical distortion lead to the emission transitions, we obtained a set of geometries between S_0- and S_1- optimized structures of **F2** using the Nudged Elastic Band (NEB) calculations and calculated the oscillator strength for each structure. As the geometry shifts from S_0 structure toward S_1, the oscillator strength increases explaining the observed emission in **Fn** series. The nudged elastic band (NEB)[28] was used as implemented in DL-FIND code[29] with the in-house developed interface to split NEB images calculations across the nodes of computational cluster.[30]

Table S18. Oscillator strengths for S0->S1 transition for a set of geometries between S_0- and S_1-optimized structures of F2 obtained from the Nudged Elastic Band (NEB) calculations.

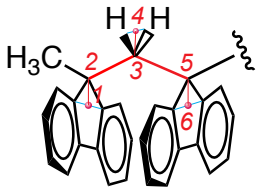


geometry	B1LYP-40/6-31G(d)	PBE0-D3/def2-SV(P)	ωB97XD/6-31G(d)
S0 (red)	0.0337	0.0187	0.0353
Green	0.0124	0.0079	0.0142
Blue	0.0029	0.0020	0.0035
Yellow	0.0000	0.0000	0.0000
S1 (magenta)	0.0000	0.0000	0.0000

S8. Probing Exciton Delocalization in F9

To probe the energetics of the exciton delocalization onto three and larger number of fluorenes (*k*) in polyfluorenes, we performed a series of single-point TD-DFT calculations of a representative polyfluorene **F9** as follows:

1. Internal structural parameters of all fluorene moieties (bond lengths and valence/dihedral angles) were set to be identical to those of **F1**^{S0};
2. Fluorenes with indices from 1 (terminal unit) to *k* were arranged in eclipsed sandwich-like arrangement by setting angles α, β, and γ:



α = *A(1-2-3) = A(3-5-6)*

β = *D(1-2-3-4) = D(4-3-5-6)*

γ = *A(2-3-5)*

   to the values identical to those in **F2**^{S1}, i.e. 128.8º, 180.0º, and 120.0º, respectively.
3. The remaining fluorenes with indices from *k*+1 to 9 were arranged in the alternant conformation of neutral polyfluorene by setting angles α, β, and γ to 132.5º, ±163.4º, and 118.2º, respectively.
4. A single-point (TD-)DFT calculation [B1LYP-40/6-31G(d)+PCM(CH_2Cl_2)] was then performed for the obtained geometry to evaluate the electronic energies of the ground and first excited states.
5. Steps 1-4 were repeated for *k* from 1 to 9.

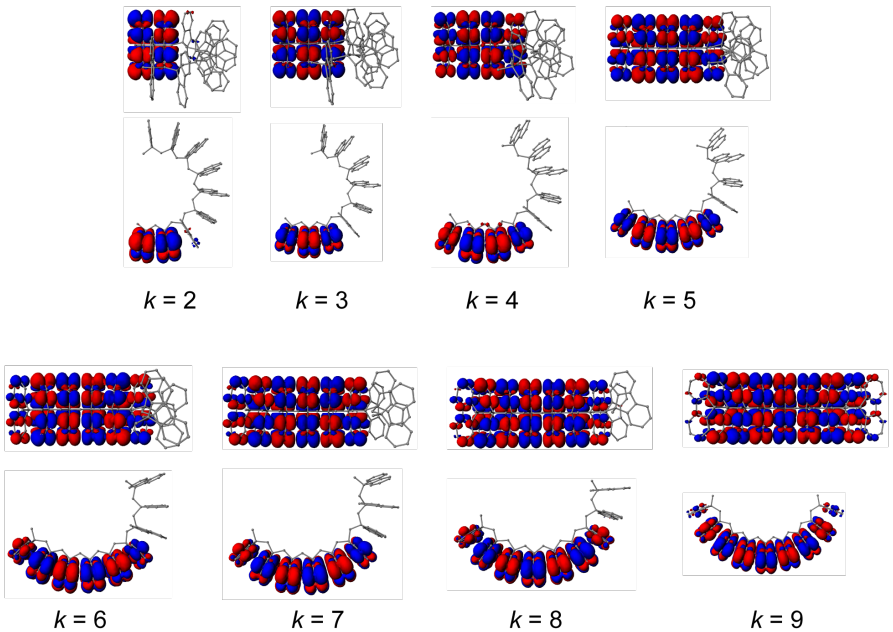


Figure S3. Transition density plots corresponding to the $S_0 \rightarrow S_1$ vertical excitation in **F9** with different number of eclipsed fluorene units (*k*).

Below is the Python script that was used to generate structures of **F9** (also available at GitHub, https://github.com/talipovm/Make-Fn):

```
#################### Make-Fn.py #####################################
#! /usr/bin/env python

# Python 2.7

import sys


ABG = {
    'S0_odd' : {'alpha':132.5,'beta':163.4,'gamma':118.2},      # ground state geometry; odd/even
are needed to create an alternant conformer
    'S0_even' : {'alpha':132.5,'beta':-163.4,'gamma':118.2},    # ground state geometry
    'S1_perfect'  :  {'alpha':120.0,'beta':180.0,'gamma':120.0},   #  make  the  planes  containing
fluorenes parallel
    'S1_normal' : {'alpha':128.8,'beta':180.0,'gamma':120.0},   # arrange fluorenes as in F2S1
    'S1_neutral' : {'alpha':132.5,'beta':180.0,'gamma':120.0}   # use alpha as in F2S0
    }

#### STRUCTURAL CONSTANTS ####

S_FIRST_ME_BRIDGE = """C
C     1    1.546
Bq    2    0.968   1      120.0
H     1    1.09    2      110.7   3        0.0
H     1    1.09    2      110.7   3        120.0
H     1    1.09    2      110.7   3        -120.0"""

S_FLUORENE = """C     %i   1.178   %i     90.0    %i       -90.0
C     %i   1.402   %i     71.4    %i       180.0
C     %i   1.390   %i     120.0   %i       180.0
C     %i   1.390   %i     120.0   %i       0.0
C     %i   1.390   %i     120.0   %i       0.0
C     %i   1.390   %i     120.0   %i       0.0
C     %i   1.178   %i     90.0    %i       90.0
C     %i   1.390   %i     71.4    %i       180.0
C     %i   1.390   %i     120.0   %i       180.0
C     %i   1.390   %i     120.0   %i       0.0
C     %i   1.390   %i     120.0   %i       0.0
C     %i   1.390   %i     120.0   %i       0.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0
H     %i   1.08    %i     120.0   %i       180.0"""

S_BRIDGE = """C    %i   1.55    %i   _(alpha)f   %i   180.0
Bq   %i   0.664   %i   _(gamma)f   %i   _(beta)f
H    %i   0.867   %i   90.0        %i   -90.0
H    %i   0.867   %i   90.0        %i   90.0
C    %i   1.55    %i   _(gamma)f   %i   180.00
Bq   %i   0.968   %i   _(alpha)f   %i   _(beta)f"""

S_LAST_ME = """C   %i   1.546   %i  120.0   %i     180.0
H   %i   1.09    %i  110.7   %i     0.0
H   %i   1.09    %i  110.7   %i     120.0
H   %i   1.09    %i  110.7   %i     240.0"""


######### FUNC ##########

def bridge(start_i,i_Bq,i_top,i_bridge):
    """
     CH2
    / \
   F   C
       |
       Bq
```

```
    New bridge unit will be constructed in the framework of CH2 (i_bridge), C (i_top), and Bq
(i_bq)
    """

    ref_ati = (
          i_top,           i_Bq,           i_bridge,
          start_i,         i_top,          i_Bq,
          start_i+1,       start_i,        i_top,
          start_i+1,       start_i,        i_top,
          start_i,         start_i+1,      i_top,
          start_i+4,       start_i,        start_i+1
    )
    D = {'s' : S_BRIDGE % ref_ati,
         'i_bridge' : start_i,
         'i_top' : start_i+4,
         'i_Bq' : start_i+5
           }
    return D


def bridge_abg(s,abg):
    """
    Inserts values of alpha, beta, and gamma
    """
    s = s.replace('_','%')
    return s % abg


def fluorene(start_i,i_Bq,i_top,i_bridge):
    """
     CH2
    / \
   F   C
       |
       Bq

    Next fluorene units will be constructed in the framework of CH2 (i_bridge), C (i_top), and Bq
(i_bq)
    """

    start_i -= 4 # calculate offset for the existing ref_ati
    i_Bq -= start_i
    i_top -= start_i
    i_bridge -= start_i

    ref_ati = (
          i_Bq,    i_top,    i_bridge,
          4,       i_Bq,     i_top,
          5,       4,        i_Bq,
          6,       5,        4,
          7,       6,        5,
          8,       7,        6,
          i_Bq,    i_top,    i_bridge,
          10,      i_Bq,     i_top,
          11,      10,       i_top,
          12,      11,       10,
          13,      12,       11,
          14,      13,       12,
          9,       8,        4,
          8,       9,        7,
          7,       8,        6,
          6,       7,        5,
          12,      13,       11,
          13,      14,       12,
          14,      15,       13,
          15,      10,       14
    )

    ati = [x + start_i for x in ref_ati]
    return S_FLUORENE % tuple(ati)
```

```
def closing_me(start_i,i_Bq,i_top,i_bridge):
    """
     CH2
    / \
       C
       |
       Bq

    Makes a close Me
    """

    ref_ati = (
        i_top,     i_Bq , i_bridge,
        start_i, i_top, i_Bq,
        start_i, i_top, i_Bq,
        start_i, i_top, i_Bq
    )

    return S_LAST_ME % ref_ati

def print_z(s):
    print s
    return len(s.split('\n'))


#########################################################
######################### MAIN ##########################
#########################################################

"""
FN = 6
Fstacked = 6
el_state = 'S1_normal'
"""

# COMMAND LINE ARGUMENTS
FN = int(sys.argv[1]) # FN, number of fluorenes
Fstacked = int(sys.argv[2]) # how many units of FN should be fully stacked?
el_state = sys.argv[3] # Determines the angle between adjacent stacked fluorene units; valid
choices are the various 'S1_*' keys in ABG


start_i = 1

# Print first Me and bridge
start_i += print_z(S_FIRST_ME_BRIDGE)

# Print first fluorene
s = fluorene(start_i=start_i,i_Bq=3,i_top=2,i_bridge=1)
start_i += print_z(s)

state_suffix = ''
i_Bq = 3
i_top = 2
i_bridge = 1

for i in range(1,FN):
    if i >= Fstacked:
        el_state = 'S0'
        if ((i - Fstacked) % 2 == 0):
            state_suffix = '_even'
        else:
            state_suffix = '_odd'

    # Print next bridge
    bridge_params = bridge(start_i=start_i,i_Bq=i_Bq,i_top=i_top,i_bridge=i_bridge)
    s = bridge_abg(bridge_params['s'],ABG[el_state+state_suffix])
    start_i += print_z(s)


    # Print next fluorene
```

```
    i_Bq=bridge_params['i_Bq']
    i_top=bridge_params['i_top']
    i_bridge=bridge_params['i_bridge']
    s = fluorene(start_i=start_i,i_Bq=i_Bq,i_top=i_top,i_bridge=i_bridge)
    start_i += print_z(s)

# Print closing Me group
s                                                                                                   =
closing_me(start_i=start_i,i_Bq=bridge_params['i_Bq'],i_top=bridge_params['i_top'],i_bridge=bridg
e_params['i_bridge'])
start_i += print_z(s)

##################### End of Make-Fn.py ######################################
```

S9. Exciton transfer coordinate in F3^{S1}

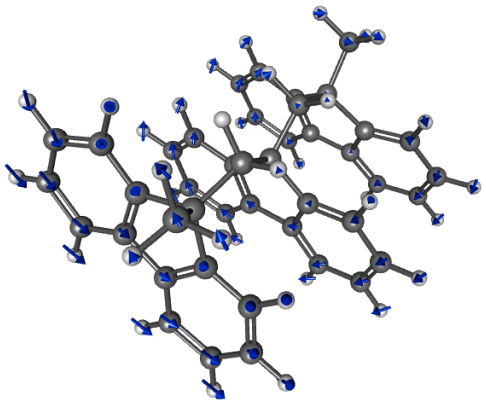


Figure **S4**. Visual representation of the low-frequency torsional mode associated with the exciton transfer coordinate along the π-stacked polyfluorenes. This mode involves the torsional motion between two fluorene units (where exciton is localized) and the adjacent fluorene unit.

Table **S19**. Frequencies of the torsional vibration mode between the pair of stacked fluorenes and the adjacent fluorene unit in **F3**^{S1}. See Figure S4 above for the visual representation.

Theory level	ω, cm^{-1}
B1LYP-40/6-31G(d)	14.9
PBE0-D3/def2-SV(P)	13.2
ωB97XD/6-31G(d)	17.1

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S11. Archive entries from the calculation files

The archive entries, formerly intended for the Browse Quantum Chemistry Database System, are organized as a simple list of data fields separated by backslash symbols, which is wrapped in 70-char text lines. The script 'Parse.Archive.pl', written in Perl, converts archive entry into human readable format. To use this script,

1. Check if Perl interpreter is installed on the system. To do this, run the command 'perl –v' in console. If console returns a message like 'command not found', please obtain and install a Perl interpreter (www.perl.org/get.html; Perl is Open Source software licensed under GNU GPL).
2. Save the script code, listed below, as a file named 'Parse.Archive.pl'.
3. Select an archive entry of interest and save it as another file (e.g. 'B-Xb.txt').
4. Run the command 'perl Parse.Archive.pl B-Xb.txt > B-Xb-parsed.txt' in console. The parsed archive entry will be stored in the file 'B-Xb-parsed.txt' in this example. In some cases, absolute path to the Perl interpreter might need to be provided.

```
# --- Parse.Archive.pl ---

# Merge all strings in one line
my $s='';
while (<>) {chomp;$s .= $_}
$_ = $s;

#     Some     PDF     viewers     (like     Mac     OS's     Preview)     might     substitute
# 'end of line' symbols by the white space symbols,
# To remove these extra white spaces, please uncomment the following lines:
# my $str_length = 70;
# my $index = $str_length;
# while (length($_) > $index) {
#     substr $_,$index,1,'';
#     $index += $str_length;
# }

# Replace all backslashes by new-line symbols
s:\\:\n:g;

# Print the resulting output
print;

# --- END ---
```

F1^{S0}

```
1\1\GINC-HPC-CN75\FOpt\RBLYP\6-31G(d)\C15H14\6498IVANOVM\19-Feb-2016\0
\\#P BLYP IOP(3/76=0600004000)/6-31G(d) opt(tight) scrf(PCM,solvent=Di
chloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine)\\
F1-S0-BLYP\\0,1\C,0.00617,0.2802,0.94954\C,0.01415,-0.36519,3.64304\C,
0.04359,-1.06268,1.35034\C,-0.02729,1.30174,1.892\C,-0.02302,0.96866,3
.24279\C,0.04784,-1.38847,2.69664\H,-0.05625,2.3386,1.58648\H,-0.04879
,1.75134,3.98795\H,0.07683,-2.42083,3.01857\H,0.01705,-0.60885,4.69618
\C,0.01041,0.32666,-0.5164\C,0.03393,-0.14723,-3.2452\C,-0.01752,1.405
82,-1.39257\C,0.05023,-0.98822,-1.00107\C,0.06208,-1.22833,-2.36521\C,
-0.00547,1.15869,-2.76167\H,-0.04809,2.42144,-1.02245\H,0.09269,-2.238
33,-2.75157\H,-0.02689,1.98688,-3.45605\H,0.0428,-0.32385,-4.31161\C,0
.07516,-1.99178,0.14415\C,-1.1574,-2.91153,0.11148\H,-1.15455,-3.52502
,-0.79002\H,-2.07991,-2.3322,0.12718\H,-1.15972,-3.58099,0.97226\C,1.3
5938,-2.8382,0.12101\H,2.24648,-2.2062,0.14388\H,1.39921,-3.45038,-0.7
8051\H,1.39388,-3.50672,0.98183\\Version=EM64L-G09RevD.01\HF=-579.7023
```

83\RMSD=4.424e-09\RMSF=3.744e-06\Dipole=0.0067991,-0.2351719,-0.007166
\Quadrupole=-7.3213299,4.3060097,3.0153202,-0.3457112,-0.0378596,-0.05
28188\PG=C01 [X(C15H14)]\\@

F1^{S1}

1\1\GINC-HPC-CN118\SP\RBLYP TD-FC\6-31G(d)\C15H14\6498IVANOVM\19-Feb-2
016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=20
0) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometh
ane,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\
\F1-S1-BLYP: emission state-specific solvation at first excited state
optimized geometry\\0,1\C,0,0.0069,0.30069,0.91033\C,0,0.01176,-0.3570
8,3.63347\C,0,0.04398,-1.08861,1.3476\C,0,-0.02696,1.34803,1.89812\C,0
,-0.02394,0.99837,3.22218\C,0,0.04612,-1.39736,2.68051\H,0,-0.05435,2.
38413,1.59371\H,0,-0.04931,1.77004,3.97951\H,0,0.0737,-2.42641,3.01322
\H,0,0.0132,-0.59369,4.68774\C,0,0.01095,0.3446,-0.47598\C,0,0.0316,-0
.13978,-3.23516\C,0,-0.0169,1.45237,-1.39579\C,0,0.05044,-1.01432,-0.9
9993\C,0,0.05989,-1.23825,-2.34963\C,0,-0.00618,1.18705,-2.73927\H,0,-
0.04561,2.46728,-1.02672\H,0,0.08886,-2.24425,-2.74657\H,0,-0.02685,2.
00506,-3.44646\H,0,0.03907,-0.30932,-4.30221\C,0,0.07614,-2.0216,0.143
25\C,0,-1.15501,-2.94453,0.11057\H,0,-1.15068,-3.55677,-0.79243\H,0,-2
.0781,-2.36675,0.12641\H,0,-1.15565,-3.6131,0.97272\C,0,1.36096,-2.868
69,0.11993\H,0,2.24741,-2.2363,0.14262\H,0,1.40027,-3.47967,-0.78306\H
,0,1.39527,-3.5361,0.9823\\Version=EM64L-G09RevD.01\HF=-579.6883079\RM
SD=4.213e-09\Dipole=0.0078375,-0.2731897,-0.0074115\Quadrupole=-7.2738
096,3.9792704,3.2945392,-0.3247723,-0.037992,-0.0872663\PG=C01 [X(C15H
14)]\\@

F1^{+*}

1\1\GINC-HPC-CN127\Stability\UBLYP\6-31G(d)\C15H14(1+,2)\6498IVANOVM\1
7-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) SCRF(PCM,solvent=D
ichloromethane) scf(fermi,xqc,maxcycle=200) int(grid=ultrafine) guess(
read) geom(check) stable(opt)\\F1N-optd\\1,2\C,0,0.0061894332,0.274674
0361,0.9230007252\C,0,0.014007121,-0.3443921292,3.6042194197\C,0,0.044
356723,-1.0921533787,1.3410317081\C,0,-0.0280863149,1.3301126095,1.864
2859114\C,0,-0.023779335,1.0079882208,3.1966149865\C,0,0.0480894322,-1
.3957339445,2.6824714319\H,0,-0.0567566194,2.358369242,1.5383898028\H,
0,-0.0491887215,1.7836647117,3.9461534848\H,0,0.0764494144,-2.41646554
8,3.0324080208\H,0,0.0165493646,-0.5697398027,4.6603463368\C,0,0.01025
88886,0.3194022377,-0.490284181\C,0,0.0336122055,-0.128885331,-3.20519
30977\C,0,-0.0187931729,1.4322551027,-1.3631288169\C,0,0.0510786204,-1
.018263554,-0.9936805321\C,0,0.0625828303,-1.2364141813,-2.351588332\C
,0,-0.0067641694,1.1950215278,-2.7131136027\H,0,-0.0495239182,2.437851
8554,-0.9730355927\H,0,0.0931408317,-2.2329807641,-2.7651994492\H,0,-0
.028002647,2.0165458155,-3.4122376185\H,0,0.0422695954,-0.2870006285,-
4.2734237412\C,0,0.0760257263,-2.0243750275,0.143084482\C,0,-1.1611529
261,-2.9404230416,0.1105310484\H,0,-1.1513602553,-3.5529642232,-0.7898
599213\H,0,-2.0846683623,-2.3641237794,0.1261141492\H,0,-1.1564253496,
-3.6086789047,0.9704253906\C,0,1.3645745875,-2.866950154,0.1201282745\
H,0,2.2528827961,-2.237944585,0.142596185\H,0,1.3972425777,-3.47882559
56,-0.7801759445\H,0,1.3921716437,-3.5345407863,0.9801094722\\Version=
EM64L-G09RevD.01\State=2-A\HF=-579.4913009\S2=0.79643\S2-1=0.\S2A=0.75
1733\RMSD=1.483e-09\Dipole=-0.0185581,0.6354214,0.0200566\Quadrupole=-
17.3249622,1.273558,16.0514042,-0.5396544,-0.1132151,-0.4697303\PG=C01
[X(C15H14)]\\@

F1^{-*}

1\1\GINC-HPC-CN121\Stability\UBLYP\6-31G(d)\C15H14(1-,2)\6498IVANOVM\17-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) SCRF(PCM,solvent=Dichloromethane) scf(fermi,xqc,maxcycle=200) int(grid=ultrafine) guess(read) geom(check) stable(opt)\\F1N-optd\\-1,2\C,0,0.0054444119,0.3000842439,0.9250366543\C,0,0.0145641283,-0.3728018882,3.6744014296\C,0,0.0434940209,-1.0648548744,1.3588227108\C,0,-0.0279984461,1.3199848968,1.919459186\C,0,-0.0227319844,0.963780997,3.2594313807\C,0,0.0480407203,-1.3949265224,2.6881651963\H,0,-0.0573103581,2.3649148508,1.6355618116\H,0,-0.0483677236,1.7471774523,4.009531193\H,0,0.0771229088,-2.434997093,2.9953629645\H,0,0.0178785637,-0.624228211,4.7261218007\C,0,0.0095217095,0.3448906506,-0.4907131838\C,0,0.0345850235,-0.1527994547,-3.2770265001\C,0,-0.018384436,1.4256367993,-1.4188300255\C,0,0.0503162341,-0.9898941679,-1.009714434\C,0,0.062572751,-1.2352475184,-2.3572198436\C,0,-0.0053423629,1.1548754917,-2.7785920238\H,0,-0.049520008,2.4505292135,-1.0695999845\H,0,0.0936118551,-2.2538168534,-2.7293973928\H,0,-0.0268042336,1.9841400672,-3.4777891172\H,0,0.0439969195,-0.3372196542,-4.3425041019\C,0,0.0750805387,-1.9920713207,0.1441040411\C,0,-1.1535772101,-2.9154490384,0.1113414546\H,0,-1.1569993643,-3.5288186878,-0.7923546705\H,0,-2.0753301823,-2.3337694589,0.1270929596\H,0,-1.1620912905,-3.5847304806,0.9744118939\C,0,1.3555476538,-2.8424629654,0.1208783655\H,0,2.2417843501,-2.2081913993,0.1435013999\H,0,1.4014806862,-3.4543971315,-0.7826300577\H,0,1.3963951244,-3.5103079431,0.9841368932\\Version=EM64L-G09RevD.01\State=2-A\HF=-579.7285426\S2=0.785587\S2-1=0.\S2A=0.750989\RMSD=5.687e-10\Dipole=0.0346,-1.1846786,-0.0373937\Quadrupole=3.4987218,6.3898983,-9.8886201,-0.0861109,0.0358798,0.515463\PG=C01 [X(C15H14)]\\@

F2^{S0}

1\1\GINC-HPC-CN109\FOpt\RBLYP\6-31G(d)\C29H24\6498IVANOVM\19-Feb-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) opt(tight) scrf(PCM,solvent=Dichloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine)\\F2-S0-BLYP\\0,1\C,-0.6990720193,0.4006096267,1.1810537654\C,-0.6222562311,-0.3889366776,3.8341536557\C,-0.2493833401,-0.8818713515,1.5183586378\C,-1.099150923,1.2953469756,2.1668686544\C,-1.0534094176,0.8924538886,3.4976280609\C,-0.2211998287,-1.283875098,2.8436474729\H,-1.4447743021,2.2870755355,1.909336113\H,-1.3616751554,1.5762495256,4.2761080963\H,0.1077098875,-2.2777031904,3.1174168498\H,-0.6013298424,-0.6926132227,4.8714667298\C,-0.679981933,0.5287225923,-0.2784468056\C,-0.5757392159,0.2127549939,-3.0258872425\C,-1.0698354312,1.5825092681,-1.0976914942\C,-0.2197805611,-0.6765885038,-0.8278175065\C,-0.1847492122,-0.8413080385,-2.2031116306\C,-1.0091581805,1.417808327,-2.4768783647\H,-1.4235048147,2.5124516484,-0.6740367299\H,0.1507428134,-1.7695745298,-2.6421069987\H,-1.308502663,2.2272837038,-3.1279519603\H,-0.541977127,0.0940118797,-4.0997559136\C,0.0852322384,-1.6897361484,0.2693210079\C,-0.9056880814,-2.8715983117,0.1599998899\H,-0.7720004988,-3.4003226244,-0.7839815085\H,-1.9345451002,-2.518105295,0.2115392733\H,-0.7484166026,-3.5831291357,0.9714468407\C,1.5123276391,-2.3063616274,0.287859142\H,1.5378223434,-3.0976781879,-0.4639526471\H,1.6041918121,-2.8209123195,1.2464378194\C,2.8094446785,-1.4756007457,0.0766381387\C,3.9870728998,-2.3762324307,0.5159580687\H,4.9400689489,-1.88305054,0.3296484281\H,3.9775288575,-3.3185048534,-0.0331683633\H,3.9215032399,-2.604322476,1.5800003179\C,3.0330842399,-1.0458112412,-1.3691273626\C,3.5715330282,0.1443180737,-3.8197638007\C,3.2472215963,0.3353443864,-1.4548995173\C,3.1085003297,-1.8343070017,-2.5054998258\C,3.3755108968,-1.2324345831,-3.7340230305\C,3.5130097779,0.9383468849,-2.6789449087\H,2.9617780956,-2.9049940332,-2.4512423601\H,3.4336302427,-1.8390239477,-4.6269635479\H,3.6761963955,2.0050746108,-2.7481723434\H,3.7777485157,0.597957

2296,-4.7791042367\C,3.1672020628,0.9004586908,-0.1055093172\C,3.03906
82704,1.4338034432,2.6068196542\C,2.9048135429,-0.1373406103,0.8002574
812\C,3.3476615563,2.2057963997,0.3384029002\C,3.2767126175,2.46644940
89,1.7021922253\C,2.8581662433,0.1266934441,2.1596707041\H,3.549064855
7,3.0057735573,-0.3607751442\H,3.4146037197,3.4758179173,2.063996548\H
,2.673277082,-0.6639280382,2.872172537\H,2.994652054,1.647702752,3.665
4635481\\Version=EM64L-G09RevD.01\HF=-1118.9098421\RMSD=5.025e-09\RMSF
=1.783e-06\Dipole=0.0376268,-0.4356553,0.0701362\Quadrupole=-12.429808
5,6.5997159,5.8300926,-2.9774766,-0.9638177,-0.1825431\PG=C01 [X(C29H2
4)]\\@

F2^{S1}

1\1\GINC-HPC-CN118\SP\RBLYP TD-FC\6-31G(d)\C29H24\6498IVANOVM\20-Feb-2
016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=20
0) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometh
ane,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\
\F2-S1-BLYP: emission state-specific solvation at first excited state
optimized geometry\\0,1\C,0,-0.3249582308,0.570413389,0.628686902\C,0,
-0.2418416536,0.4358482646,3.4125134505\C,0,-0.0514237338,-0.665063747
9,1.2928174751\C,0,-0.5406285893,1.7439598631,1.3904454495\C,0,-0.4929
37317,1.6605601899,2.7636712265\C,0,-0.0484631592,-0.7323573847,2.6676
217721\H,0,-0.7529055794,2.6844466773,0.9019283892\H,0,-0.6540530632,2
.5483773655,3.3598173763\H,0,0.1338014305,-1.6696606955,3.1758659029\H
,0,-0.2277287928,0.3957555524,4.4920409964\C,0,-0.4007160556,0.3373741
273,-0.7702170558\C,0,-0.610085449,-0.6916777452,-3.3529560421\C,0,-0.
7178047352,1.2047996409,-1.8431033894\C,0,-0.1764493896,-1.0509233531,
-1.0239978512\C,0,-0.3171400229,-1.5592735617,-2.295497628\C,0,-0.8152
543367,0.6810026416,-3.1123740382\H,0,-0.8950994716,2.2560067347,-1.66
50310227\H,0,-0.172558591,-2.6136299975,-2.4892966858\H,0,-1.056076281
1,1.3305767256,-3.9427684998\H,0,-0.7094710797,-1.0790862512,-4.356581
0288\C,0,0.1192909114,-1.7877234893,0.2767038952\C,0,-0.9194025256,-2.
9005173924,0.5175128573\H,0,-0.8514314575,-3.6676993955,-0.2545564295\
H,0,-1.9295012069,-2.4935487437,0.5049105981\H,0,-0.7572708735,-3.3800
248299,1.4834662258\C,0,1.5250455483,-2.4427717772,0.3096866099\H,0,1.
5372050294,-3.2297543515,-0.4488784012\H,0,1.6289075731,-2.9471508609,
1.2739041958\C,0,2.7938934129,-1.5755693117,0.1003262589\C,0,4.0168992
748,-2.5097599192,0.1837673804\H,0,4.9398640531,-1.9487397686,0.044102
1595\H,0,3.9679611631,-3.281859792,-0.5848381623\H,0,4.062153456,-3.00
39109086,1.1548696002\C,0,2.7951175589,-0.8082584939,-1.2161004178\C,0
,2.8725630081,0.9916360721,-3.3426933985\C,0,2.8343286064,0.599174868,
-0.9722069466\C,0,2.8402155252,-1.2947967121,-2.5028465479\C,0,2.85088
15266,-0.3973696589,-3.575718837\C,0,2.8668891008,1.5001571294,-2.0635
012838\H,0,2.8346621281,-2.3596929164,-2.6927264442\H,0,2.872727752,-0
.7695115307,-4.5897542567\H,0,2.9020075333,2.567007281,-1.8937624478\H
,0,2.8960734331,1.6666547351,-4.1872730223\C,0,2.909740888,0.824618746
8,0.4280411295\C,0,3.2159452236,0.6928905822,3.1959473472\C,0,2.921043
214,-0.4349497606,1.1027323898\C,0,3.0402776865,2.0212600869,1.1730055
121\C,0,3.1882083142,1.9386272312,2.5390836425\C,0,3.1093131329,-0.494
9951479,2.464984565\H,0,3.0382595246,2.980708261,0.67532638\H,0,3.2878
549563,2.8435946792,3.1227098753\H,0,3.1425925206,-1.4467969189,2.9778
988904\H,0,3.350478109,0.6565635721,4.2673013842\\Version=EM64L-G09Rev
D.01\HF=-1118.8864601\RMSD=3.931e-09\Dipole=0.0457868,-0.4638594,0.073
8403\Quadrupole=-13.2349755,7.3087015,5.926274,-2.7828277,1.5751182,-0
.047205\PG=C01 [X(C29H24)]\\@

F2^{+*}

1\1\GINC-HPC-CN11\Stability\UBLYP\6-31G(d)\C29H24(1+,2)\TALIPOVM\12-Ma

r-2013\0\\#P blyp/6-31G(d) IOP(3/76=0600004000) stable(opt) pop(npa) S
CRF(check) guess(read) geom(allcheck) nosym int(grid=ultrafine) scf(fe
rmi,xqc,maxcyc=200)\\Title\\1,2\C,0,-0.4248284211,0.5584706179,0.65147
42434\C,0,-0.3390150502,0.4309120647,3.4077369133\C,0,-0.0997117216,-0
.6591743185,1.2957053187\C,0,-0.6820534717,1.7208102956,1.3928572015\C
,0,-0.6317032883,1.6471060709,2.7694181076\C,0,-0.0819689925,-0.725657
5838,2.6755199869\H,0,-0.9295823514,2.648457152,0.8982268445\H,0,-0.82
97770811,2.525193662,3.3657965673\H,0,0.138388234,-1.6497089849,3.1899
528216\H,0,-0.3226162709,0.391991499,4.48704776\C,0,-0.5011741655,0.32
40165653,-0.7664127196\C,0,-0.7021369074,-0.6855015143,-3.3282525283\C
,0,-0.8535540072,1.1904255524,-1.8113852843\C,0,-0.2249881661,-1.04142
73219,-1.0152737205\C,0,-0.3509190985,-1.5492453905,-2.29374043\C,0,-0
.9460816638,0.6766445165,-3.088314099\H,0,-1.0625712527,2.2323317307,-
1.618966197\H,0,-0.1707050552,-2.5940339251,-2.501317995\H,0,-1.219602
3797,1.3196462794,-3.911543931\H,0,-0.7979494326,-1.0697903309,-4.3331
666432\C,0,0.1037162084,-1.7721754577,0.2780546553\C,0,-0.9146186285,-
2.9060047625,0.5188194403\H,0,-0.8323008214,-3.6653467827,-0.258013650
8\H,0,-1.9321086751,-2.5190256533,0.513498944\H,0,-0.7352255984,-3.386
555678,1.4799473029\C,0,1.5213914801,-2.4096508251,0.3042409454\H,0,1.
5308221535,-3.1976613912,-0.4506130941\H,0,1.6263828225,-2.9177295931,
1.2642097141\C,0,2.8081759328,-1.5629571814,0.0949985141\C,0,4.0115686
105,-2.5244014922,0.1828723558\H,0,4.9471500245,-1.9851553774,0.045204
9903\H,0,3.9435679724,-3.2949377472,-0.584370363\H,0,4.0395078159,-3.0
178929897,1.1536865287\C,0,2.8442254968,-0.7992508528,-1.2203834636\C,
0,3.0082622508,0.9957430675,-3.3465122376\C,0,2.9346717781,0.594358545
6,-0.99127812\C,0,2.8770655412,-1.2901173444,-2.5112193804\C,0,2.94953
87929,-0.3893592368,-3.5709996997\C,0,3.006532632,1.497735377,-2.06153
32692\H,0,2.8354378403,-2.3516645866,-2.7079016144\H,0,2.9704030777,-0
.7610508633,-4.584963557\H,0,3.0753299299,2.5607627761,-1.8839918284\H
,0,3.067286896,1.6678153056,-4.1896077846\C,0,3.0106320714,0.824204588
6,0.4275038113\C,0,3.3111721112,0.702744879,3.169283941\C,0,2.97042489
66,-0.4249608768,1.0916538235\C,0,3.1753013668,2.0175850925,1.14546334
63\C,0,3.3195353308,1.9457433607,2.515583502\C,0,3.1462314086,-0.48481
06385,2.4605286709\H,0,3.2034680311,2.9697281979,0.6365163665\H,0,3.45
20717572,2.8481941316,3.0935042334\H,0,3.144169206,-1.4295282562,2.984
7392859\H,0,3.4437608308,0.6691556284,4.2407154743\\Version=EM64L-G09R
evC.01\HF=-1118.7058027\S2=0.773284\S2-1=0.\S2A=0.750527\RMSD=3.388e-0
9\Dipole=-0.0289018,0.2912117,-0.043771\Quadrupole=-11.48111,-1.779254
5,13.2603645,-1.3008867,1.5512254,2.6373727\PG=C01 [X(C29H24)]\\@

F2^{-*}

1\1\GINC-HPC-CN109\Stability\UBLYP\6-31G(d)\C29H24(1-,2)\TALIPOVM\26-M
ar-2016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) stable(opt) pop(nbo)
scrf(check) guess(read) geom(allcheck) nosym scf(fermi,xqc,maxcyc=200)
int(grid=ultrafine)\\Title\\-1,2\C,0,-0.5222574194,0.5461991077,0.739
3200048\C,0,-0.3478248937,0.3415238685,3.5242013245\C,0,-0.1307189756,
-0.666869998,1.3508112328\C,0,-0.8000613002,1.6679119548,1.5421656794\
C,0,-0.7078435121,1.5500497864,2.9217671315\C,0,-0.0632905974,-0.77618
32367,2.7223561518\H,0,-1.0950439189,2.6079038298,1.0940582442\H,0,-0.
9236708626,2.4103400935,3.5434308159\H,0,0.2179051653,-1.7131556403,3.
1870987875\H,0,-0.2905195071,0.2665818717,4.6013553178\C,0,-0.61010454
52,0.3461182743,-0.6853729866\C,0,-0.7859680146,-0.6181117486,-3.30536
94513\C,0,-1.0063226235,1.2088755069,-1.7232297319\C,0,-0.2793598501,-
0.9964860042,-0.9837734533\C,0,-0.3841156339,-1.4786462571,-2.26951454
23\C,0,-1.083533573,0.7164578993,-3.0183197046\H,0,-1.2596920878,2.240
7577712,-1.5167899471\H,0,-0.1479731429,-2.5119097605,-2.4910833093\H,
0,-1.3892608604,1.3773910416,-3.8201161514\H,0,-0.8625040535,-0.986810

322,-4.3188503221\C,0,0.0940923534,-1.7437206436,0.2932412879\C,0,-0.8
939586104,-2.9070448234,0.521082304\H,0,-0.8129540885,-3.6504670462,-0
.2738051001\H,0,-1.9196264324,-2.5394364314,0.5372381418\H,0,-0.698114
1926,-3.4065835355,1.4715141239\C,0,1.5197650001,-2.3609846279,0.29624
95516\H,0,1.5232879876,-3.1523442821,-0.4592169441\H,0,1.6387657182,-2
.8690540763,1.2578645712\C,0,2.8085820864,-1.5236078792,0.0685773415\C
,0,3.9970078868,-2.5021616584,0.1819654458\H,0,4.9393087258,-1.9783420
359,0.0241151217\H,0,3.9219757997,-3.2967684243,-0.5623813017\H,0,4.02
82049072,-2.9661584588,1.1692660416\C,0,2.869971083,-0.8018780536,-1.2
741958778\C,0,3.1020530228,0.8852237442,-3.4683144753\C,0,3.030283359,
0.5890752098,-1.0782296798\C,0,2.861386808,-1.3394051262,-2.5423910715
\C,0,2.976155536,-0.4936056442,-3.6572382234\C,0,3.1336961612,1.437873
0497,-2.1955043431\H,0,2.7586979875,-2.407803772,-2.6869322956\H,0,2.9
638243948,-0.9067244474,-4.6564053081\H,0,3.2499717199,2.5064065266,-2
.0683817014\H,0,3.1841459495,1.5347521972,-4.3311047368\C,0,3.11509985
41,0.8553735082,0.3366778855\C,0,3.3696730276,0.7881821412,3.121702652
5\C,0,3.007692499,-0.3660570115,1.0421935042\C,0,3.332844677,2.0488448
924,1.0484726879\C,0,3.4521497375,1.9990729611,2.4304001096\C,0,3.1512
065286,-0.404135084,2.4111466277\H,0,3.4170952876,2.9942366873,0.52828
45512\H,0,3.6202468925,2.9160756108,2.9817512248\H,0,3.0855336068,-1.3
434672154,2.9456727291\H,0,3.475084933,0.7676457108,4.1975700647\\Vers
ion=EM64L-G09RevD.01\HF=-1118.9346065\S2=0.769868\S2-1=0.\S2A=0.75038\
RMSD=3.177e-09\Dipole=0.1503222,-1.3374734,0.2024806\Quadrupole=-15.21
77554,16.4503094,-1.232554,-4.6467279,1.7834433,-2.6770418\PG=C01 [X(C
29H24)]\\@

F3^{S0}

1\1\GINC-HPC-CN118\FOpt\RBLYP\6-31G(d)\C43H34\6498IVANOVM\19-Feb-2016\
0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) opt(tight) scrf(PCM,solvent=D
ichloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine)\
\F3-S0-BLYP\\0,1\C,1.4928141592,-0.2792163792,1.3983295633\C,1.8051245
977,-1.9959055257,3.5481536639\C,0.9146148593,-1.5539308466,1.36664375
\C,2.2167197284,0.1459821996,2.5064389605\C,2.3663986882,-0.7211195378
,3.5838290636\C,1.0787736528,-2.4188523937,2.4363035906\H,2.6629931515
,1.1306154403,2.533121946\H,2.9278557502,-0.4062629464,4.4523359749\H,
0.652876194,-3.4133788128,2.4193758675\H,1.9368601131,-2.6636638014,4.
3880731816\C,1.2195626378,0.3844631335,0.1213954735\C,0.572989023,1.12
02250967,-2.4656168542\C,1.6208308186,1.6295703867,-0.3500561958\C,0.4
763842946,-0.4868422825,-0.6882519258\C,0.1710422362,-0.1261873873,-1.
990786795\C,1.2865657452,1.99474261,-1.6490731281\H,2.1929828491,2.300
5785121,0.2758505471\H,-0.3828782779,-0.7924899127,-2.6352154516\H,1.5
90800812,2.9591929707,-2.0313218541\H,0.3274511552,1.4108237036,-3.477
3982902\C,0.2302460289,-1.8107761169,0.0274876597\C,1.008603663,-2.925
5371892,-0.7124769864\H,2.0680461321,-2.6803207569,-0.771695324\H,0.62
87285472,-3.0514434402,-1.7265057461\H,0.9076429069,-3.8786004035,-0.1
918547942\C,-2.3849505445,0.8887214387,1.2090651853\C,-1.6376046878,0.
4261529664,3.8315639191\C,-2.1976528801,-0.4259257659,1.6609256353\C,-
2.1972117147,1.9710283475,2.0613343725\C,-1.8219974984,1.7302738998,3.
3777671248\C,-1.8230935547,-0.6556267719,2.9746680464\H,-2.3410627456,
2.983621164,1.7102194015\H,-1.6728817029,2.5604017842,4.0543222097\H,-
1.6748972061,-1.6596342873,3.3407623504\H,-1.3463378036,0.2507729478,4
.8575483993\C,-2.7783648981,0.8510880951,-0.20076688\C,-3.482289351,0.
2198658305,-2.8031992495\C,-3.0795334458,1.8758646225,-1.0891791428\C,
-2.8281505356,-0.4858002402,-0.6079879308\C,-3.1795874315,-0.805377640
1,-1.9089787018\C,-3.4322527427,1.550825754,-2.3949758229\H,-3.0423320
018,2.9102960028,-0.7763277583\H,-3.2221058292,-1.8352173752,-2.239380
8288\H,-3.6696529966,2.336931181,-3.0982639541\H,-3.7579976279,-0.0196

312168,-3.8208567348\C,-2.4590938812,-1.4227729899,0.5384216081\C,-1.2
346454744,-2.3230585203,0.1586079414\H,-1.4980490251,-2.8013977664,-0.
7864801211\H,-1.1861498838,-3.1348673656,0.8856111115\C,-5.4785823577,
-0.6941148249,3.3806997671\C,-4.4487954185,-2.4014368348,5.3018329874\
C,-4.8751102426,-1.8977790331,2.9970982912\C,-5.5602820422,-0.33513295
33,4.7213201858\C,-5.0368245574,-1.1962579558,5.6802254826\C,-4.369111
2973,-2.7590034435,3.9570536396\H,-6.025801528,0.5942681139,5.01937180
41\H,-5.09291335,-0.9320186453,6.7269774298\H,-3.9155527326,-3.7008508
982,3.6777199121\H,-4.0544208392,-3.0663552701,6.057525646\C,-5.977296
7072,-0.0227225103,2.1783000308\C,-6.8454554049,0.7438390267,-0.333565
1602\C,-6.6886472327,1.1639844314,2.0396316931\C,-5.678710152,-0.81834
87058,1.0626039202\C,-6.1315615613,-0.4439748478,-0.1923002592\C,-7.11
58973508,1.5457800865,0.7730934249\H,-6.9169753653,1.7766840921,2.9009
491594\H,-5.9282885006,-1.0537535639,-1.0600027391\H,-7.6702249781,2.4
654337947,0.6474934186\H,-7.1916243457,1.0457475166,-1.3120724881\C,-4
.9667495064,-2.0983640486,1.4875291085\C,-3.6063701847,-2.4520429387,0
.8170563568\H,-3.8289331462,-2.9172739907,-0.1447847055\H,-3.189170567
5,-3.2519069513,1.4302318217\C,-5.9039324306,-3.2994294419,1.212332399
4\H,-5.4535530557,-4.2290304257,1.5623354186\H,-6.0986528805,-3.398269
3252,0.1442915779\H,-6.8566562678,-3.1688308682,1.7235357997\\Version=
EM64L-G09RevD.01\HF=-1658.1135841\RMSD=6.444e-09\RMSF=1.477e-06\Dipole
=-0.0386964,-0.5764304,-0.2422831\Quadrupole=-15.2484335,8.8742551,6.3
741783,1.2446028,7.9354318,-0.9847277\PG=C01 [X(C43H34)]\\@

F3^{S1}

1\1\GINC-HPC-CN77\SP\RBLYP TD-FC\6-31G(d)\C43H34\6498IVANOVM\21-Feb-20
16\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=200
) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometha
ne,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\\
F3-S1-BLYP: emission state-specific solvation at first excited state o
ptimized geometry\\0,1\C,0,1.0724739428,0.2052076724,0.927704351\C,0,1
.5374440046,-0.6461834813,3.5420747374\C,0,0.7597067253,-1.1293784324,
1.3276446894\C,0,1.6109801568,1.1120104579,1.8716982275\C,0,1.83269105
28,0.6757672658,3.1589613947\C,0,1.0267837698,-1.5554784615,2.60769600
42\H,0,1.8580313191,2.1237919387,1.5823018797\H,0,2.2420458375,1.35746
93542,3.8921235344\H,0,0.8141712853,-2.5724579025,2.9089694662\H,0,1.7
380127279,-0.9677352143,4.5538447732\C,0,0.8277259182,0.3411912576,-0.
4649625542\C,0,0.3596083051,0.0098285199,-3.1937574587\C,0,1.048526436
7,1.4256620348,-1.3477070367\C,0,0.3534929666,-0.904638696,-0.97899060
35\C,0,0.1631397954,-1.0747525496,-2.3304614172\C,0,0.8107581772,1.245
5577754,-2.6918299959\H,0,1.4130739652,2.3721905801,-0.9740371002\H,0,
-0.1708503749,-2.023885178,-2.7277280481\H,0,0.9735135478,2.0649435092
,-3.3787980531\H,0,0.1995156961,-0.1099451753,-4.255507921\C,0,0.22010
91706,-1.9240492151,0.1451463152\C,0,1.1178305269,-3.1470703343,-0.132
1242654\H,0,2.1508008805,-2.837023213,-0.2835154966\H,0,0.7871038281,-
3.6777740289,-1.025603701\H,0,1.0916094295,-3.8462294853,0.7044594776\
C,0,-2.0949232458,0.7375270669,1.5456951323\C,0,-1.7627040443,-0.07245
97203,4.1873028417\C,0,-2.173164662,-0.646581002,1.8962428071\C,0,-1.8
610284375,1.7088492919,2.5479358233\C,0,-1.7022600297,1.2929309719,3.8
496810901\C,0,-2.0195977337,-1.0363803154,3.2068336573\H,0,-1.81639181
05,2.7582272983,2.2934048103\H,0,-1.5209014918,2.0214713218,4.62797985
7\H,0,-2.0786763139,-2.077770421,3.4855899709\H,0,-1.6438371851,-0.374
2146472,5.2176977151\C,0,-2.3183193692,0.8806283926,0.1522556868\C,0,-
2.9116473453,0.6071260527,-2.5559685284\C,0,-2.3889309391,2.0339471565
,-0.6658651663\C,0,-2.5491942231,-0.4081979026,-0.4151474692\C,0,-2.86
45996878,-0.5347462379,-1.7489655093\C,0,-2.6848594978,1.881864404,-2.
0007553976\H,0,-2.2254896304,3.0157613225,-0.2448200816\H,0,-3.0462324

897,-1.5068553708,-2.1875937495\H,0,-2.7407887359,2.7521777687,-2.6401
739201\H,0,-3.1513888415,0.5158724271,-3.6053845542\C,0,-2.4179347529,
-1.4920926372,0.6511547855\C,0,-1.2233371923,-2.4555451265,0.355903727
8\H,0,-1.4874950988,-3.0324006973,-0.534465565\H,0,-1.1789487034,-3.17
10077211,1.1804703546\C,0,-5.5218973584,-0.9912580936,3.4432967334\C,0
,-4.8485754843,-3.1660186437,5.0197920426\C,0,-5.0396243683,-2.1641611
89,2.8503014129\C,0,-5.6605599631,-0.8976328119,4.8232244241\C,0,-5.31
54827955,-1.9927598191,5.6087951888\C,0,-4.7132980758,-3.2580206985,3.
6353982348\H,0,-6.0312587182,0.0079648336,5.2834626612\H,0,-5.41677951
47,-1.9356299815,6.6835466875\H,0,-4.3553676645,-4.1768904438,3.190015
496\H,0,-4.5930155864,-4.0131597709,5.6408648008\C,0,-5.8289295856,-0.
0296532916,2.3821887133\C,0,-6.3552616019,1.3485393098,0.0424740269\C,
0,-6.3661869311,1.2507432101,2.4554707639\C,0,-5.5348025578,-0.6179390
369,1.1432032186\C,0,-5.8159796289,0.0655952277,-0.0289520815\C,0,-6.6
229192935,1.939193633,1.27533291\H,0,-6.5911102352,1.702911691,3.41165
18289\H,0,-5.6119296211,-0.3774384034,-0.9922305631\H,0,-7.0404800747,
2.9356193332,1.3142892292\H,0,-6.5670131169,1.8899268754,-0.8688782609
\C,0,-5.0291697423,-2.0443047715,1.3297818825\C,0,-3.6673955814,-2.430
6023073,0.682439964\H,0,-3.8641593998,-2.6943525409,-0.3576773903\H,0,
-3.3724773262,-3.3659272585,1.1608891664\C,0,-6.0781040712,-3.02670000
75,0.7557266897\H,0,-5.7738499964,-4.0596701888,0.9290637446\H,0,-6.19
19143936,-2.8828370229,-0.3188351102\H,0,-7.0480849424,-2.8736885065,1
.2267540685\\Version=EM64L-G09RevD.01\HF=-1658.0904251\RMSD=4.568e-09\
Dipole=-0.626297,-0.4794327,-0.0347728\Quadrupole=-16.8217229,9.293324
8,7.5283982,2.0127817,3.6095699,-0.9751387\PG=C01 [X(C43H34)]\\@

F4^{S0}

1\1\GINC-HPC-CN70\FOpt\RBLYP\6-31G(d)\C57H44\6498IVANOVM\19-Feb-2016\0
\\#P BLYP IOP(3/76=0600004000)/6-31G(d) opt(tight) scrf(PCM,solvent=Di
chloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine)\\
F4-S0-BLYP\\0,1\C,1.2652376331,0.0012157425,1.7552194419\C,1.530010904
3,-1.8986632892,3.7517737665\C,0.8385907763,-1.3117051253,1.5329726804
\C,1.825505124,0.3697969208,2.9718769047\C,1.9545403517,-0.5900462809,
3.9703564683\C,0.9699960974,-2.264746362,2.5292724606\H,2.1557914775,1
.38466726,3.1458123034\H,2.3876456545,-0.3186454042,4.9231203638\H,0.6
455356151,-3.2854248807,2.3727467286\H,1.6359231189,-2.6356982579,4.53
57485139\C,1.0021210808,0.7819625655,0.5454222862\C,0.3154893733,1.798
5142275,-1.9326284341\C,1.247468792,2.1224880897,0.2713026808\C,0.4138
959936,-0.0551417744,-0.414292212\C,0.0751092443,0.4552845537,-1.65659
03331\C,0.8978138609,2.6265630814,-0.9758178409\H,1.7014739373,2.76500
89187,1.0131967373\H,-0.3758152375,-0.1725196862,-2.4086205083\H,1.079
7541054,3.6674762028,-1.2050559439\H,0.0477785407,2.2006200625,-2.8994
526147\C,0.2632725824,-1.4715661508,0.1282481677\C,-2.6311223918,1.007
9167774,1.4569958378\C,-1.8979059617,0.4125645603,4.056095972\C,-2.321
4172214,-0.314065314,1.810204113\C,-2.5785784763,2.0302561234,2.397292
7799\C,-2.208195105,1.7233358434,3.7013176461\C,-1.9579308431,-0.61051
52217,3.1135439179\H,-2.8201665661,3.0478751396,2.1226097322\H,-2.1600
231023,2.5069589067,4.444825831\H,-1.7172427471,-1.620629447,3.4050937
177\H,-1.6100373128,0.1850820494,5.0727217219\C,-2.9848925293,1.046840
8146,0.0370610426\C,-3.5531045756,0.5645539676,-2.629660982\C,-3.35888
27385,2.1068633648,-0.7791563783\C,-2.8959164686,-0.2517438023,-0.4739
365032\C,-3.1801654249,-0.4966969551,-1.8070874193\C,-3.642129917,1.85
70689922,-2.1178798813\H,-3.4287214517,3.1118124487,-0.3860184896\H,-3
.1167828795,-1.4962283326,-2.2176292815\H,-3.9333132334,2.6719693267,-
2.7660769463\H,-3.7757859163,0.3831161932,-3.6720516657\C,-2.475645698
4,-1.2409587613,0.609928468\C,-1.1977365344,-2.0431888833,0.1789662149
\H,-1.4306467463,-2.429831763,-0.8134794938\H,-1.1335506161,-2.9227715

501,0.8198950371\C,-5.6510105353,-0.8611411903,3.3492524301\C,-4.58062
8772,-2.5761726372,5.2414675106\C,-4.9461733035,-2.000634985,2.9431695
15\C,-5.8126673489,-0.5687004226,4.6987293742\C,-5.2690713405,-1.43334
82326,5.6431612305\C,-4.4192526323,-2.8661338447,3.8878106935\H,-6.356
5664694,0.3110083185,5.0144159535\H,-5.3876662521,-1.2209292917,6.6965
002696\H,-3.8875187287,-3.7600175513,3.5893345539\H,-4.1713726664,-3.2
451519204,5.9855912627\C,-6.1529072629,-0.1773655252,2.1552197546\C,-6
.985260431,0.6256687534,-0.3575825927\C,-6.9453675791,0.9589169304,2.0
343886224\C,-5.7568509599,-0.9026160101,1.0222260565\C,-6.1922930182,-
0.5125311447,-0.2338562016\C,-7.3541092611,1.3598751716,0.7676853387\H
,-7.2496588571,1.517533036,2.9089187051\H,-5.914525746,-1.0711290257,-
1.1151779537\H,-7.9699444573,2.2413973772,0.655748819\H,-7.3174926362,
0.9414695884,-1.3365076451\C,-4.9645886114,-2.1417268755,1.4243220362\
C,-3.5576447296,-2.3618210364,0.7934803414\H,-3.7110183077,-2.79266440
13,-0.1976437188\H,-3.1053132497,-3.1586985695,1.3853009071\C,-5.79471
76319,-3.3975936155,1.0633847973\H,-5.2882204937,-4.3044973339,1.39576
35696\H,-5.9399650791,-3.4661393366,-0.0148430994\H,-6.773710066,-3.36
05288189,1.5390502807\C,3.6208334006,-0.5362217264,-2.2453636957\C,2.2
79331488,-0.6964731605,-4.6621925155\C,2.6239313928,-1.501634283,-2.43
05874574\C,3.9426321547,0.3576544057,-3.2605133122\C,3.2610981892,0.27
34574042,-4.4702287808\C,1.9593073139,-1.591330863,-3.6427971774\H,4.7
124058881,1.1038814966,-3.1192954312\H,3.5000304064,0.960548428,-5.269
9092627\H,1.1990381613,-2.3434861495,-3.8072363053\H,1.7640910523,-0.7
576989141,-5.6106149635\C,4.1989333557,-0.7178665295,-0.9120362825\C,5
.0414519712,-1.5655264771,1.5827030046\C,5.2461492664,-0.0501355434,-0
.2866218168\C,3.5547470353,-1.7944405737,-0.285238596\C,3.9911308024,-
2.2314500805,0.955193355\C,5.6598340762,-0.4780341858,0.9696128906\H,5
.7411294132,0.7803395682,-0.7710688663\H,3.5214128447,-3.0720662653,1.
4438206754\H,6.4730935525,0.0295342594,1.4694018305\H,5.3784753823,-1.
8961588985,2.5550912428\C,2.5041357439,-2.4048913956,-1.2069779633\C,1
.0475794017,-2.563610784,-0.6788693941\H,1.0230047783,-3.4643343515,-0
.0627052997\H,0.4541701863,-2.8051109669,-1.5616686008\C,2.967509921,-
3.8270277642,-1.6074539799\H,3.9542971866,-3.7943764326,-2.0670362497\
H,2.2735481392,-4.2729620101,-2.3209269533\H,3.0179793543,-4.475900504
3,-0.7329275144\\Version=EM64L-G09RevD.01\HF=-2197.3167941\RMSD=1.286e
-09\RMSF=1.789e-06\Dipole=-0.1018065,-0.726263,-0.2135097\Quadrupole=-
18.2529957,9.5516706,8.7013251,2.0217395,10.4483257,-2.4291771\PG=C01
[X(C57H44)]\\@

F4^{S1}

1\1\GINC-HPC-CN125\SP\RBLYP TD-FC\6-31G(d)\C57H44\6498IVANOVM\22-Feb-2
016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=20
0) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometh
ane,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\
\F4-S1-BLYP: emission state-specific solvation at first excited state
optimized geometry\\0,1\C,0,1.4075246498,0.0090055426,1.3292164313\C,0
,1.793364955,-1.8607579609,3.3574741314\C,0,0.9007857937,-1.3183377112
,1.1995478687\C,0,2.1144065791,0.3832593518,2.4975202619\C,0,2.2943612
539,-0.551062296,3.4911360314\C,0,1.0763163736,-2.23142677,2.214838842
1\H,0,2.4931730704,1.3891092625,2.6102794513\H,0,2.8330011897,-0.28211
80578,4.3894226907\H,0,0.6927518072,-3.2393694142,2.1295477307\H,0,1.9
411137449,-2.5738253291,4.1555146662\C,0,1.022226451,0.7622197003,0.19
16346397\C,0,-0.0033375884,1.790990593,-2.1803714043\C,0,1.2451463992,
2.1218017799,-0.1316390008\C,0,0.2605171262,-0.0677934824,-0.689842906
6\C,0,-0.2518210725,0.4531238812,-1.85531356\C,0,0.7295357018,2.616370
6806,-1.3069258191\H,0,1.8049908419,2.7587559534,0.5382918722\H,0,-0.8
331053353,-0.1591800365,-2.5280941636\H,0,0.8925761639,3.6521300225,-1

.5715518235\H,0,-0.4076251515,2.2039398266,-3.0929664618\C,0,0.177850038,-1.4860356295,-0.1346341584\C,0,-2.6865884594,1.0343391572,1.0435141747\C,0,-1.6072702258,0.8726213167,3.5831313023\C,0,-2.272753226,-0.2080003853,1.547809582\C,0,-2.5570039675,2.1936566511,1.799801658\C,0,-2.0124548538,2.1044642409,3.0752547385\C,0,-1.7373948608,-0.287447007,2.822990881\H,0,-2.8732270347,3.1496193671,1.4055889537\H,0,-1.9033002269,2.9961272,3.676953009\H,0,-1.4148145136,-1.2320756906,3.2312918101\H,0,-1.1856816706,0.8139033746,4.5765918735\C,0,-3.2092931344,0.8445813968,-0.310005992\C,0,-4.0165027356,-0.0481926318,-2.8035211757\C,0,-3.7203306037,1.7573912565,-1.2241285703\C,0,-3.1085439196,-0.5118769378,-0.6337662431\C,0,-3.5090848779,-0.9617893137,-1.8810965938\C,0,-4.1238005777,1.3013739557,-2.4750743213\H,0,-3.799170075,2.8067742992,-0.9754995366\H,0,-3.4351265766,-2.0078831927,-2.1485891383\H,0,-4.5205174444,1.9997369946,-3.1988229837\H,0,-4.3310107117,-0.3899793923,-3.7798588845\C,0,-2.5162838189,-1.3114260438,0.5241111034\C,0,-1.2470687067,-2.1070695778,0.0537997892\H,0,-1.5313874075,-2.5763459075,-0.8883512893\H,0,-1.1005240964,-2.9336182531,0.7484134328\C,0,-5.4433935353,-0.6118590814,3.4582218311\C,0,-4.0722568493,-1.8870305408,5.4984097376\C,0,-4.6987787943,-1.7663561299,3.1877027871\C,0,-5.4940124709,-0.0838759203,4.7434372236\C,0,-4.7995430772,-0.7282500211,5.762057054\C,0,-4.0214893023,-2.4126850569,4.2087493708\H,0,-6.0676047101,0.8081812454,4.9545138377\H,0,-4.8305635418,-0.331298438,6.767109826\H,0,-3.4568016689,-3.3158228777,4.0183777861\H,0,-3.5453008045,-2.3838225401,6.3010357417\C,0,-6.1093608592,-0.1908532301,2.2230302341\C,0,-7.2441764735,0.0799475827,-0.2856398521\C,0,-6.9933602569,0.8565890979,1.9878168948\C,0,-5.7714039592,-1.0902891981,1.2015008454\C,0,-6.3563735561,-0.9667731636,-0.0484310032\C,0,-7.5545659032,0.9896994141,0.7229551385\H,0,-7.2521613124,1.5504943726,2.7758120157\H,0,-6.1245672096,-1.6637462329,-0.8401066051\H,0,-8.2443393887,1.7979325003,0.52350954\H,0,-7.6953715432,0.1871033829,-1.2620618198\C,0,-4.8517100474,-2.1859599355,1.7291758543\C,0,-3.4988684848,-2.4361082077,0.9992236387\H,0,-3.714504443,-3.0369703691,0.1133989085\H,0,-2.9388380277,-3.0956079873,1.6634577067\C,0,-5.6129945413,-3.5332418831,1.6871900819\H,0,-5.0098966039,-4.3317580403,2.1209156625\H,0,-5.8516522441,-3.8086721207,0.6597817564\H,0,-6.5437126772,-3.4662248674,2.2487234356\C,0,3.6851394214,-0.296995344,-1.359419904\C,0,2.7623685877,0.6652508471,-3.8088372173\C,0,2.7405548797,-1.0423819952,-2.1276970594\C,0,4.1476288191,0.9522292312,-1.8378138193\C,0,3.6808675255,1.413167687,-3.0489709035\C,0,2.3182563692,-0.5823579922,-3.3527952828\H,0,4.8670191982,1.52549265,-1.2700316784\H,0,4.0242234936,2.3666193664,-3.4270293724\H,0,1.6212190526,-1.1551356105,-3.9498139612\H,0,2.4260937085,1.0413528483,-4.7642407672\C,0,4.0546952335,-1.05569243,-0.2161639522\C,0,4.5526128492,-3.0050768111,1.7155287238\C,0,5.0068475708,-0.8039533915,0.8005295913\C,0,3.348895908,-2.2973778754,-0.2323042189\C,0,3.6262875679,-3.2703571649,0.6996325639\C,0,5.2401297055,-1.7771716447,1.7467612576\H,0,5.5539243098,0.1281177792,0.8219306949\H,0,3.1127864703,-4.2222338848,0.6758766875\H,0,5.9648463006,-1.5993484966,2.5297765308\H,0,4.7680443494,-3.7583383238,2.4595411042\C,0,2.410402545,-2.3563989079,-1.4308546325\C,0,0.910011045,-2.5108959552,-1.0625050562\H,0,0.791014257,-3.4982438526,-0.6082197626\H,0,0.3559233916,-2.5393082502,-2.0036358071\C,0,2.7773381757,-3.5491309033,-2.3374114531\H,0,3.8226029681,-3.4935906108,-2.6380056802\H,0,2.1638073342,-3.5555150849,-3.2390467126\H,0,2.6224519826,-4.4950724169,-1.8172404412\\Version=EM64L-G09RevD.01\HF=-2197.2937371\RMSD=4.478e-09\Dipole=-0.8845625,-0.3752285,0.1040598\Quadrupole=-20.6846932,12.6735852,8.0111081,3.330271,15.6632354,-1.5387027\PG=C01 [X(C57H44)]\\@

F4’S1

1\1\GINC-HPC-CN128\SP\RBLYP TD-FC\6-31G(d)\C57H44\6498IVANOVM\21-Feb-2
016\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=20
0) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometh
ane,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\
\F4m-S1-BLYP: emission state-specific solvation at first excited state
optimized geometry\\0,1\C,0,1.2592770089,1.0714874596,1.1872266093\C,
0,2.0918233309,-0.0801984404,3.5842586726\C,0,1.0744955277,-0.32188987
92,1.427148248\C,0,1.8692384804,1.8810922346,2.1753833484\C,0,2.273103
1993,1.2972404126,3.3544820135\C,0,1.4642561603,-0.8805385649,2.622068
8291\H,0,2.0031441056,2.9408286073,2.0101820282\H,0,2.7434122732,1.901
4191177,4.118348583\H,0,1.3227739179,-1.9355773841,2.8154973506\H,0,2.
4080503406,-0.5128456571,4.5223315684\C,0,0.6977547232,1.4008234261,-0
.0732920153\C,0,-0.566477369,1.5241949981,-2.5500547976\C,0,0.58549392
98,2.6454680291,-0.7369542292\C,0,0.1473004636,0.2224493395,-0.6675012
595\C,0,-0.4895650665,0.2955433579,-1.8839254018\C,0,-0.0444940626,2.6
902844108,-1.9592598356\H,0,0.9816213159,3.5442358489,-0.2858407837\H,
0,-0.9136725748,-0.5860023156,-2.3410825609\H,0,-0.1360044604,3.632785
1093,-2.4818085986\H,0,-1.0669717712,1.5861741566,-3.5053454758\C,0,0.
3945208204,-0.9831833948,0.2317502251\C,0,-3.0016413991,1.1483510841,1
.1268211823\C,0,-1.9206244634,1.704980464,3.6114322591\C,0,-2.24810950
2,0.1724321815,1.7959451078\C,0,-3.199325645,2.4059263597,1.6862786363
\C,0,-2.6479630726,2.6800628949,2.9326974714\C,0,-1.7235864287,0.44527
65917,3.0492113188\H,0,-3.779058522,3.1575822378,1.1683228218\H,0,-2.7
914227597,3.6530704457,3.3815410981\H,0,-1.1546348804,-0.2985526653,3.
5865284942\H,0,-1.5035513349,1.9265714554,4.5837705148\C,0,-3.50991197
64,0.5752619868,-0.1213897291\C,0,-4.25133412,-0.9898927091,-2.2820937
525\C,0,-4.3182385288,1.1233444432,-1.1105033552\C,0,-3.0648659902,-0.
7489193219,-0.2128348383\C,0,-3.4437228347,-1.5380232692,-1.2867497937
\C,0,-4.6822377483,0.3322573238,-2.1954050467\H,0,-4.6619147712,2.1463
760925,-1.0425274147\H,0,-3.1216374678,-2.5682334796,-1.3628099471\H,0
,-5.3094025589,0.7441663912,-2.9736418737\H,0,-4.5490921333,-1.5969019
796,-3.1256491832\C,0,-2.2451639124,-1.1365346203,1.0137587618\C,0,-0.
8741697738,-1.7884207412,0.6683502424\H,0,-1.0911478834,-2.5218671865,
-0.1097605333\H,0,-0.5665099275,-2.3762967987,1.5341111966\C,0,-3.0394
827356,-2.1965493501,1.814552344\C,0,3.5079536734,0.4848207015,-1.5009
433245\C,0,2.2845207751,0.6011740595,-4.0024604704\C,0,2.7464446734,-0
.616932973,-1.9902796521\C,0,3.6466440635,1.650515098,-2.2922626892\C,
0,3.0377748312,1.691349601,-3.5258193531\C,0,2.1664386693,-0.564777052
9,-3.2363004102\H,0,4.2316713688,2.4874085822,-1.9378662338\H,0,3.1319
488936,2.5757669332,-4.1411558667\H,0,1.5925139032,-1.3985333827,-3.61
8301873\H,0,1.8253040309,0.6535386045,-4.9789446894\C,0,4.0637564891,0
.138287176,-0.2424924176\C,0,4.9367256953,-1.0360548742,2.126197978\C,
0,4.9258414451,0.8599452334,0.6166819572\C,0,3.6629086765,-1.190566333
5,0.1011767887\C,0,4.1114825001,-1.7686572792,1.2653189225\C,0,5.35034
12391,0.2648094677,1.7824691673\H,0,5.2497976496,1.8575267505,0.355660
7352\H,0,3.8198526622,-2.7732767953,1.5330403125\H,0,6.0070420153,0.80
37086892,2.45186303\H,0,5.2927293049,-1.4867793071,3.0411018967\C,0,2.
7426345173,-1.7553307205,-0.9743243602\C,0,1.3051844099,-2.0626144848,
-0.4405487797\H,0,1.4043482649,-2.8773567297,0.2807840986\H,0,0.741811
135,-2.469182085,-1.283908379\C,0,6.7556264837,-2.2809081047,-1.644809
1192\C,0,6.5111725753,-0.6801917923,-3.8865656311\C,0,5.6035308641,-2.
3650592462,-2.4409045479\C,0,7.7755162461,-1.3882379784,-1.9551037976\
C,0,7.642724406,-0.5826617249,-3.0802209423\C,0,5.4905175034,-1.576256
2926,-3.5746262528\H,0,8.6621212807,-1.3246470101,-1.3392692058\H,0,8.
4257440333,0.1177323405,-3.3353880544\H,0,4.6184803501,-1.6368735804,-
4.2082756509\H,0,6.4220084495,-0.0545611182,-4.7635564104\C,0,6.659059
5348,-3.272489484,-0.5718175645\C,0,6.008680769,-5.3104730867,1.186327

2065\C,0,7.5429666297,-3.5930688885,0.451779392\C,0,5.4480170132,-3.96
01536207,-0.7136871155\C,0,5.1249423525,-4.9878445353,0.1574790529\C,0
,7.2071553633,-4.6153713127,1.333629183\H,0,8.4776811902,-3.061212098,
0.5648120037\H,0,4.2001129606,-5.5393261176,0.0508504907\H,0,7.8835440
459,-4.8763300523,2.1355453863\H,0,5.7635979269,-6.1086696764,1.873010
8209\C,0,4.6776432476,-3.4661654726,-1.9342505163\C,0,3.1945354634,-3.
1034257263,-1.6273706691\H,0,2.8185715971,-3.9203232452,-1.0094724874\
H,0,2.639890167,-3.1779910941,-2.5635818346\C,0,4.6388345289,-4.606350
1264,-2.9800151046\H,0,-3.1092699594,-3.1300870065,1.2547752155\H,0,-4
.0500240252,-1.8465964501,2.0207512483\H,0,-2.5485268229,-2.4069155063
,2.7648926577\H,0,4.2085702934,-4.2530119336,-3.9172546851\H,0,4.03171
19186,-5.4381445942,-2.6205292373\H,0,5.6420328038,-4.9791530463,-3.18
20387183\\Version=EM64L-G09RevD.01\HF=-2197.2942307\RMSD=1.902e-09\Dip
ole=-0.233056,-0.6232593,-0.0744185\Quadrupole=-14.1453198,8.894721,5.
2505988,5.1524966,13.2997032,-4.2310622\PG=C01 [X(C57H44)]\\@

F5^{S0}

1\1\GINC-HPC-CN49\FOpt\RBLYP\6-31G(d)\C71H54\6498IVANOVM\20-Dec-2015\0
\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=Di
chloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine) f
req\\F5-not-opt\\0,1\C,1.0466362501,0.6001542995,1.7784254885\C,1.5224
446593,-1.2556987632,3.7773336516\C,0.856471578,-0.7625403716,1.528351
4472\C,1.4746533567,1.0405001508,3.0246429212\C,1.711239826,0.10216911
31,4.0238608241\C,1.0930274418,-1.6932886113,2.5260754182\H,1.62208990
39,2.0937704435,3.2202141419\H,2.044493951,0.4291402505,4.9990981587\H
,0.9497890161,-2.7513765793,2.3485248982\H,1.7101209561,-1.975225248,4
.5622997402\C,0.7205736526,1.3422257273,0.5594034676\C,-0.0085640459,2
.2638911745,-1.9433314238\C,0.7494274348,2.7089148765,0.3057645796\C,0
.3304690318,0.4317109114,-0.4336132625\C,-0.0395150271,0.8963317314,-1
.6849062787\C,0.3828447139,3.1643911261,-0.9550348246\H,1.0505684863,3
.4079706944,1.0738952797\H,-0.3467556613,0.2127605812,-2.4604826049\H,
0.4007742425,4.2239235157,-1.1700665932\H,-0.2923920434,2.6286953393,-
2.9202727234\C,0.375292754,-0.995992552,0.098773658\C,-2.9373309793,1.
0191572401,1.5315364118\C,-2.2509180735,0.3270091844,4.1203311209\C,-2
.3864297151,-0.2431710403,1.7951294986\C,-3.1265687933,1.9430613716,2.
5534788176\C,-2.7726919031,1.5904342418,3.8506747373\C,-2.0630115588,-
0.5968249892,3.0951181405\H,-3.5516599495,2.9161022952,2.3488143813\H,
-2.9127267759,2.2970894794,4.6568185034\H,-1.6570144902,-1.5716937737,
3.3198744015\H,-1.9889110054,0.0601386592,5.13449457\C,-3.2870879699,1
.091486958,0.1109436642\C,-3.8430422467,0.667295326,-2.5683283706\C,-3
.8954939128,2.1026181556,-0.6243102979\C,-2.9457905495,-0.125433079,-0
.4912825851\C,-3.2329636078,-0.3443437282,-1.8287804908\C,-4.168075348
6,1.8831885024,-1.9706019945\H,-4.1597084462,3.043360583,-0.1611301638
\H,-2.9912588969,-1.2860670125,-2.3037963959\H,-4.642001759,2.65892372
89,-2.5556712625\H,-4.0690474954,0.5058250308,-3.6131163891\C,-2.35922
06684,-1.0946751432,0.5303125917\C,-1.0087676988,-1.7345315584,0.09155
2969\H,-1.1837777678,-2.0916478453,-0.9241723781\H,-0.8682544044,-2.63
53827404,0.6915566134\C,-3.3499532409,-2.2713702805,0.7064145666\C,3.4
788305487,0.4229838259,-2.1171758933\C,2.1840899672,0.1243525732,-4.54
60094332\C,2.7293586975,-0.7290192103,-2.3733845309\C,3.5809054438,1.4
301598646,-3.0684027706\C,2.9278118863,1.2731187268,-4.2863808249\C,2.
0816496934,-0.8822882008,-3.587900716\H,4.1593730062,2.3223469905,-2.8
714690372\H,2.9987595651,2.0475924365,-5.0375268539\H,1.4983412195,-1.
7684194244,-3.8027471183\H,1.6818005996,0.0131859771,-5.497051259\C,4.
0550080118,0.3090397858,-0.7769455694\C,4.9008432193,-0.3762739789,1.7
63645611\C,4.8746056605,1.1864483803,-0.0763981607\C,3.6553745494,-0.9
12173187,-0.2141087683\C,4.0801092199,-1.2526368098,1.0594438332\C,5.2

954760427,0.8350465589,1.2005820839\H,5.1810787488,2.1264389741,-0.514
4648616\H,3.7853990893,-2.1865995088,1.5101400795\H,5.9335301741,1.505
3783446,1.759899826\H,5.2341861014,-0.6405209186,2.7571462552\C,2.7653
063584,-1.6834378467,-1.1822315302\C,1.3141199474,-1.995310058,-0.6659
932398\H,1.3844387721,-2.8662455498,-0.0137387579\H,0.7706820313,-2.33
94698049,-1.5465710783\C,6.6949459372,-2.0040179815,-2.0800785008\C,6.
1706616466,-0.9961771883,-4.6007867711\C,5.5554203039,-2.4295791603,-2
.778964181\C,7.5701328912,-1.0775082608,-2.634999709\C,7.3000945801,-0
.5754203305,-3.9025596114\C,5.2964915795,-1.9251515345,-4.0427451182\H
,8.4479537965,-0.7524498683,-2.0935485278\H,7.9704678435,0.1459201304,
-4.349126614\H,4.4268452721,-2.2400989402,-4.59733799\H,5.9694074613,-
0.5993219864,-5.5857318398\C,6.7406591019,-2.6902464925,-0.7880738885\
C,6.3512648508,-4.2344090826,1.47679935\C,7.6575973401,-2.6109459782,0
.2525673393\C,5.6320721378,-3.5378645308,-0.7010640742\C,5.4345352167,
-4.3122048954,0.4301531227\C,7.4549620525,-3.389248749,1.3873289539\H,
8.5155371347,-1.9559737819,0.1871048368\H,4.5823942054,-4.9744625577,0
.5128318382\H,8.1592275402,-3.3381159131,2.2061207644\H,6.2050230036,-
4.8346841675,2.3641339208\C,4.7786715675,-3.4574368888,-1.9640944346\C
,3.2897865899,-3.0992397196,-1.6181268342\H,3.0074946106,-3.8054610327
,-0.837185303\H,2.6812316121,-3.3700670023,-2.4811077652\C,7.497172265
2,-4.7787399239,-4.9069485906\C,5.7841714417,-4.3805844754,-7.04574416
43\C,6.128005664,-5.0342100848,-4.7649184664\C,8.0121124273,-4.3123538
268,-6.111238145\C,7.1446194797,-4.1112502008,-7.1798190218\C,5.270692
9034,-4.8469922047,-5.8369190545\H,9.0692662144,-4.1138102275,-6.22262
05242\H,7.529746014,-3.7504573262,-8.1233183337\H,4.2130759033,-5.0576
98304,-5.7481581795\H,5.1220674735,-4.2298112576,-7.8869478252\C,8.165
966824,-5.1297825423,-3.6520072099\C,8.9504025362,-6.0651382535,-1.169
5175738\C,9.5143821693,-5.1056730677,-3.313126373\C,7.2041158696,-5.59
98103205,-2.7459283736\C,7.600193226,-6.0877204217,-1.5110212457\C,9.9
000577819,-5.5715665133,-2.0614529459\H,10.2546555317,-4.7420945219,-4
.012567591\H,6.8758559236,-6.4720013515,-0.808435126\H,10.9443999859,-
5.5597141014,-1.7820594357\H,9.263036406,-6.4336982812,-0.2026514725\C
,5.8181091729,-5.5993945008,-3.382077359\C,4.6579036229,-4.8651232066,
-2.6461918753\H,4.2868728384,-5.5396554094,-1.8724462317\H,3.854489156
4,-4.8035469544,-3.3813075513\C,5.3528323358,-7.0664256427,-3.55119768
42\H,6.0760619215,-7.6339360014,-4.1350824467\H,4.3911165516,-7.110230
276,-4.0638116961\H,5.2416751479,-7.5493030388,-2.5802033599\H,-3.4076
16305,-2.8677454888,-0.2049214852\H,-4.3485274841,-1.9018684188,0.9352
404227\H,-3.0316030488,-2.9244132594,1.5191660469\\Version=EM64L-G09Re
vD.01\HF=-2736.5198827\RMSD=6.289e-09\RMSF=6.170e-07\Dipole=-0.4188106
,-0.7664878,-0.0125288\Quadrupole=-17.4159324,5.8322865,11.5836459,7.1
83523,13.2742175,-6.9464224\PG=C01 [X(C71H54)]\\@

F5^{S1}

1\1\GINC-HPC-CN62\SP\RBLYP TD-FC\6-31G(d)\C71H54\6498IVANOVM\03-Apr-20
16\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=200
) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometha
ne,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\\
F5-S1-BLYP: emission state-specific solvation at first excited state o
ptimized geometry\\0,1\C,0,1.2947021051,1.0727767399,1.1718916868\C,0,
2.1482982032,-0.074149061,3.564252253\C,0,1.1187664235,-0.3211552187,1
.4133561442\C,0,1.9063058298,1.8855530947,2.1563021246\C,0,2.320486392
3,1.3039526183,3.3332044108\C,0,1.5186108992,-0.8777171626,2.605651043
1\H,0,2.0334599496,2.9460569063,1.9904292778\H,0,2.7921766361,1.910947
3623,4.0940489532\H,0,1.3839874225,-1.9335546202,2.7997844963\H,0,2.47
2151781,-0.505096627,4.5005195023\C,0,0.7238170919,1.3987977689,-0.085
6282021\C,0,-0.5564174489,1.5145939976,-2.5550868772\C,0,0.6001042584,

2.6424693648,-0.748864634\C,0,0.17661556,0.2175023246,-0.6764227596\C,
0,-0.4679473143,0.2865115716,-1.888929216\C,0,-0.0380383733,2.68351815
59,-1.9673199271\H,0,0.9934245114,3.5437924184,-0.3003064088\H,0,-0.88
96538778,-0.5976980497,-2.3432056939\H,0,-0.1384053748,3.6256134568,-2
.4890840925\H,0,-1.0635119539,1.5734574812,-3.5071109215\C,0,0.4354326
424,-0.9862284257,0.2220541803\C,0,-2.9693500488,1.1289659765,1.129058
2243\C,0,-1.8794612855,1.6967359912,3.6072453981\C,0,-2.2067684858,0.1
588528423,1.79633774\C,0,-3.1719839745,2.3863252869,1.6871889749\C,0,-
2.6162739847,2.6660436624,2.930430654\C,0,-1.6774324748,0.4372445401,3
.0463381022\H,0,-3.7587517889,3.1335066087,1.170677976\H,0,-2.76355410
73,3.6389465672,3.3782622769\H,0,-1.1007782274,-0.3019824274,3.5818129
356\H,0,-1.4588156047,1.9227455511,4.5770218247\C,0,-3.479880931,0.550
5871248,-0.1157756444\C,0,-4.22171312,-1.0228342204,-2.2703704436\C,0,
-4.2956049477,1.0921308741,-1.1023690416\C,0,-3.0275145828,-0.77114550
87,-0.2068082461\C,0,-3.4066307295,-1.5644396201,-1.2775368985\C,0,-4.
6598239215,0.2969678884,-2.1842209385\H,0,-4.6448346761,2.1133088067,-
1.0348322662\H,0,-3.0788970332,-2.5929158779,-1.3531302534\H,0,-5.2926
939653,0.7038452547,-2.9604908218\H,0,-4.5196716739,-1.6331138552,-3.1
115092976\C,0,-2.2000905907,-1.1516147078,1.0168236358\C,0,-0.82723763
5,-1.7969728001,0.6668952125\H,0,-1.0444053643,-2.5336960324,-0.108081
9097\H,0,-0.5125883926,-2.3808472518,1.5328411766\C,0,-2.9852655865,-2
.2142264733,1.8232580912\C,0,3.5276126921,0.4879545251,-1.5279390168\C
,0,2.2868638477,0.6077527959,-4.0195178521\C,0,2.7707680066,-0.6172170
202,-2.0164399727\C,0,3.6536755594,1.6582605054,-2.3146169683\C,0,3.03
6328818,1.7008357588,-3.5436423648\C,0,2.1812914851,-0.5623351626,-3.2
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,2.5885025916,-4.1557335222\H,0,1.6093334691,-1.3971857148,-3.64035804
32\H,0,1.8203466944,0.6614197897,-4.9924659014\C,0,4.0930434017,0.1413
767,-0.2745480502\C,0,4.9779763781,-1.0236377723,2.0918321806\C,0,4.95
16110093,0.8703231206,0.5821178804\C,0,3.7051511302,-1.1920809249,0.06
74287646\C,0,4.1586013914,-1.7645191713,1.2321586433\C,0,5.3819808996,
0.2797968219,1.7477707675\H,0,5.266263364,1.8705064288,0.3197739295\H,
0,3.8795051317,-2.7724126419,1.5000563817\H,0,6.0349943146,0.823979887
5,2.4164633957\H,0,5.338505108,-1.4717049081,3.0062346873\C,0,2.779605
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746377\H,0,1.4524239192,-2.8759527333,0.268798966\H,0,0.7753607906,-2.
4741287625,-1.2914648264\C,0,6.7093033458,-2.2873360819,-1.6199306858\
C,0,6.4720022267,-0.5970056362,-3.7943939813\C,0,5.6022623042,-2.40105
65727,-2.4745628365\C,0,7.6951714518,-1.3345179915,-1.8484195597\C,0,7
.568257891,-0.4871079619,-2.9425346628\C,0,5.4878993441,-1.5559376389,
-3.5662553292\H,0,8.5465848558,-1.2500220296,-1.1871354359\H,0,8.32466
17103,0.2615525407,-3.1334393612\H,0,4.6458223423,-1.6261080784,-4.236
1538921\H,0,6.382524522,0.0666536662,-4.6427440059\C,0,6.5894299985,-3
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C,0,7.4127952742,-3.560951545,0.5285798635\C,0,5.40935225,-4.005123332
4,-0.75966985\C,0,5.0417434395,-5.0048490038,0.1258776596\C,0,7.040529
3274,-4.5656104574,1.4159958332\H,0,8.3260494766,-3.0043270096,0.68799
66878\H,0,4.131071471,-5.5719126206,-0.0174664127\H,0,7.6690648817,-4.
7909460871,2.2663609954\H,0,5.5829158648,-6.0595118632,1.9156415863\C,
0,4.6795753984,-3.5228006487,-2.0108734543\C,0,3.2031778505,-3.1124874
474,-1.6715639723\H,0,2.8125749472,-3.9236645084,-1.056426183\H,0,2.62
91892329,-3.1571860979,-2.5965530639\C,0,7.5580422742,-4.3106295689,-4
.9666961256\C,0,6.1109908239,-3.2008866897,-7.0502244451\C,0,6.1664563
61,-4.4571124876,-5.009197013\C,0,8.2290064301,-3.6014945154,-5.956544
448\C,0,7.4944459572,-3.0437152949,-6.9978868095\C,0,5.4412706795,-3.9
120945488,-6.0561882674\H,0,9.3039466208,-3.4877631086,-5.9256813865\H
,0,8.0013300739,-2.4904859237,-7.7761522174\H,0,4.3673002292,-4.031490

6077,-6.1118496813\H,0,5.5529307794,-2.77064694,-7.8700839813\C,0,8.06
52008703,-5.041805402,-3.8031846541\C,0,8.5166275526,-6.6712075463,-1.
6135389946\C,0,9.3690146744,-5.2394438494,-3.3621823275\C,0,6.98261640
08,-5.6365142926,-3.1391207968\C,0,7.2112403431,-6.4700339023,-2.05610
00069\C,0,9.5872397305,-6.0542323257,-2.2572364308\H,0,10.2026185099,-
4.7786011767,-3.8741675848\H,0,6.3913511084,-6.9534495163,-1.545842439
1\H,0,10.5948519384,-6.2186178163,-1.9014780077\H,0,8.6994219634,-7.31
1363988,-0.7619534963\C,0,5.6733983009,-5.3283074738,-3.857950555\C,0,
4.5092333126,-4.6902879371,-3.0432350246\H,0,4.0096383185,-5.496327046
3,-2.5022729628\H,0,3.7898046401,-4.3597159243,-3.7934507971\C,0,5.110
7899156,-6.6438922445,-4.4481475539\H,0,5.8413511346,-7.1136637196,-5.
1051536067\H,0,4.2057717879,-6.4525912582,-5.0259451155\H,0,4.86287884
27,-7.3471881584,-3.6530039232\H,0,-3.0523344785,-3.1493286534,1.26573
23629\H,0,-3.996843063,-1.869366063,2.0329523374\H,0,-2.4892033763,-2.
4199166125,2.7719604298\\Version=EM64L-G09RevD.01\HF=-2736.4974052\RMS
D=3.109e-09\Dipole=-0.1713381,-0.7738241,-0.0893209\Quadrupole=-13.038
1424,7.8862444,5.151898,6.6717785,15.8749397,-8.5013745\PG=C01 [X(C71H
54)]\\@

F6^{S0}

1\1\GINC-HPC-CN126\FOpt\RBLYP\6-31G(d)\C85H64\6498IVANOVM\19-Dec-2015\
0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) Opt(tight) SCRF(PCM,solvent=D
ichloromethane) nosym scf(fermi,xqc,maxcycle=200) int(grid=ultrafine)
freq\\F6N-optd\\0,1\C,1.0507320716,0.6174238728,1.7928379348\C,1.55626
36535,-1.2139459162,3.8067444176\C,0.8526532336,-0.7474968087,1.563261
4848\C,1.5006707829,1.0722876699,3.0259133211\C,1.7519702405,0.1464168
805,4.0329937188\C,1.1052359867,-1.6661043071,2.5683659024\H,1.6529039
66,2.1277108567,3.2056455894\H,2.1018216176,0.484956917,4.9984440504\H
,0.9576467253,-2.7261864163,2.4067954397\H,1.7556543847,-1.9241303191,
4.5973445091\C,0.7016907801,1.3452238953,0.5718860073\C,-0.0752705296,
2.2401102291,-1.9255503921\C,0.7318656295,2.7084475561,0.3011215397\C,
0.2855987808,0.4245128701,-0.4011717385\C,-0.1044817782,0.8758413184,-
1.651087735\C,0.3402156541,3.1508105431,-0.9567844882\H,1.0532589818,3
.4148954451,1.0541854247\H,-0.4300925574,0.1850153163,-2.4121139021\H,
0.3575994815,4.2077283891,-1.1846122904\H,-0.3788325771,2.5942459846,-
2.9004206212\C,0.3467360651,-0.9976843507,0.1444810781\C,-2.9061329443
,1.0034758037,1.4678824721\C,-2.1255919149,0.4885216281,4.0692984364\C
,-2.4116663689,-0.263881454,1.8103905749\C,-3.0078719964,2.0133870556,
2.4179357899\C,-2.6129176139,1.7469160599,3.7234490062\C,-2.0259473704
,-0.5207394541,3.1156671781\H,-3.3885143946,2.9893518355,2.1497138896\
H,-2.6847089513,2.520626599,4.4753854249\H,-1.6458976894,-1.4888692033
,3.4003603204\H,-1.8213400169,0.2918130978,5.0875326572\C,-3.248348703
5,1.0081721078,0.0448488612\C,-3.7222602495,0.4805048431,-2.6314697519
\C,-3.7672940388,2.0124359382,-0.7627705841\C,-2.9643865139,-0.2563580
45,-0.4800446395\C,-3.2013378487,-0.5240389509,-1.818099598\C,-4.00247
35872,1.7399350843,-2.1064000356\H,-3.9867375107,2.9912060321,-0.35881
71252\H,-2.9883213589,-1.4979238222,-2.2396577343\H,-4.4060551311,2.51
10252359,-2.7479206226\H,-3.9100217338,0.2807917414,-3.6773917084\C,-2
.4090174759,-1.1857539921,0.5961468269\C,-1.0178207585,-1.7780582304,0
.1706714165\H,-1.1807898476,-2.180262351,-0.8294960608\H,-0.8300939269
,-2.6470248562,0.8015697891\C,-5.6154083285,-1.3841711212,3.3339445069
\C,-4.2816815302,-2.9582998078,5.1806470862\C,-4.7361048113,-2.3826145
742,2.8981944571\C,-5.8225507414,-1.1616931308,4.6906205581\C,-5.14622
9861,-1.9543949008,5.6121400413\C,-4.0759720028,-3.1787653672,3.819915
4639\H,-6.5013822115,-0.3910031853,5.0290908573\H,-5.2975653718,-1.795
0097901,6.6706071638\H,-3.4066534317,-3.9657617232,3.4982100665\H,-3.7
693947196,-3.5737578136,5.906942461\C,-6.22009375,-0.7547420021,2.1577

069444\C,-7.1742642247,-0.0243526125,-0.3339150019\C,-7.1876248308,0.2
398755003,2.0667741337\C,-5.7099610125,-1.3706931326,1.005611966\C,-6.
2032747364,-1.0188037489,-0.2405309282\C,-7.6573051381,0.6060911485,0.
8107312185\H,-7.5790910657,0.7146027577,2.9560269433\H,-5.8369318876,-
1.4966982903,-1.1369191035\H,-8.4098820787,1.3771999568,0.7221948579\H
,-7.5546656641,0.261244677,-1.3045723436\C,-4.7316568125,-2.4803461043
,1.3757657434\C,-3.3069897685,-2.4633983363,0.7469773547\H,-3.39049790
23,-2.8884712346,-0.2547977016\H,-2.7393589166,-3.1962374599,1.3217685
143\C,-5.3559560238,-3.8396985829,0.9756627195\H,-4.7144340595,-4.6656
323227,1.2851990668\H,-5.4876246973,-3.8990503372,-0.1048842165\H,-6.3
291555007,-3.9693668722,1.4469341478\C,3.4458661438,0.4428187265,-2.08
71299682\C,2.1395045129,0.1537912929,-4.5109086279\C,2.692508091,-0.70
66257128,-2.343001475\C,3.5454703922,1.4526327649,-3.0358905474\C,2.88
65438051,1.3004104021,-4.2512955886\C,2.0391644703,-0.8551680191,-3.55
51008643\H,4.1274879929,2.3426144685,-2.839415554\H,2.9559131331,2.076
7869736,-5.000631989\H,1.4531305294,-1.7395015139,-3.769886875\H,1.632
8523274,0.0462804128,-5.460058565\C,4.0332542011,0.3209248736,-0.75247
11963\C,4.9058629668,-0.3822905875,1.7741394497\C,4.8614138593,1.19267
43084,-0.055014625\C,3.637775686,-0.9033218375,-0.1931853406\C,4.07618
09674,-1.2529141324,1.0732224633\C,5.2957804494,0.8323509606,1.2149981
619\H,5.1646858109,2.1349878404,-0.4903202239\H,3.7856015145,-2.189746
6,1.5207096603\H,5.9407799318,1.4981535654,1.7717520934\H,5.249780852,
-0.6536234385,2.7621163335\C,2.7375641117,-1.667575229,-1.1574058139\C
,1.2913899372,-1.9873355466,-0.630233601\H,1.3726424403,-2.8598334691,
0.0186838535\H,0.7445705601,-2.3318186433,-1.5085068339\C,6.6768145861
,-2.0000485994,-2.04841333\C,6.1628326818,-0.9312156036,-4.5455704861\
C,5.5326191498,-2.3984691647,-2.7558658064\C,7.561549941,-1.0704866771
,-2.5827446885\C,7.2966429028,-0.5375772705,-3.8387374133\C,5.27916398
59,-1.8635269127,-4.0081962255\H,8.4425146758,-0.76648115,-2.034214420
5\H,7.974188304,0.1867593347,-4.2693365986\H,4.406039302,-2.1563940789
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081\PG=C01 [X(C85H64)]\\@

F6^{S1}

1\1\GINC-HPC-CN61\SP\RBLYP TD-FC\6-31G(d)\C85H64\6498IVANOVM\03-Apr-20
16\0\\#P BLYP IOP(3/76=0600004000)/6-31G(d) scf(fermi,xqc,maxcycle=200
) int(grid=ultrafine) scrf(PCM,ExternalIteration,solvent=Dichlorometha
ne,read) nosym td(singlets,nstates=3,root=1) geom(check) guess(read)\\
F6-S1-BLYP: emission state-specific solvation at first excited state o
ptimized geometry\\0,1\C,0,1.1691766391,0.8531108786,1.2567567331\C,0,
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