Supporting Information

A Highly Fluorescent Dinuclear Aluminium Complex with Near-Unity Quantum Yield

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1. Additional Figures

**Figure S1.** The crystal packing of 1 in the unit cell (fragments have been completed), viewed along the a axis. Adjacent layers containing molecules pointing in the same direction are given in green and pink, respectively.

**Figure S2.** The crystal packing of 1 in the unit cell (fragments have been completed), viewed along the b axis. Adjacent layers containing molecules pointing in the same direction are given in green and pink, respectively.
Figure S3. The crystal packing of 1 in the unit cell (fragments have been completed), viewed along the c axis. Adjacent layers containing molecules pointing in the same direction are given in green and pink, respectively.

Figure S4. $C_2$ equilibrium structure of 1 (hydrogen atoms omitted for clarity) at the B3LYP10/def2svp/SMD(toluene) level of theory. Selected bond lengths [Å] and angles [°]: Al1–N1' 1.9267, Al1–O1 1.9131, Al1–C17 1.9677, Al1–C18 1.9625, N1'–Al1–O1 92.5, C17–Al1–C18 122.3.
Figure S5. Cyclic voltammogram of 1 (2 mM) in MeCN/TBA[PF$_6$] (0.1 M) vs. Fc/FC$^+$; $v = 0.1$ V s$^{-1}$.

$U_{ox} = 0.38$ V

$U_{red} = -2.205$ V

$\Delta U = 57$ mV

Figure S6. a) Absorption and b) normalized emission spectra of complex 1 (1.4 µM) in acetonitrile (black), dichloromethane (red) and toluene (blue).
Figure S7. Photoluminescence decay curve (spectrally integrated) and instrument response function for 1 in oxygen free toluene. A single exponential decay with a lifetime of 2.3 ns is observed.

Figure S8. Fluorescence lifetime image for a crystal of 1.
Figure S9. Photoluminescence decay curvefit for a crystal of 1 (Figure S8).

Figure S10. Photographs (on blue background) of electrospun fleeces of a) pure polystyrene and b) polystyrene containing 10 % (w/w) of complex 1.

Figure S11. SEM micrograph of pure non-woven polystyrene fabric, i.e. not containing complex 1.
Figure S12. EDX investigation of polystyrene fibers containing 10 % (w/w) of complex 1. a) EDX spectrum; b) EDX mapping.

Figure S13. Absorption (black) and emission spectra (red, excitation at 410 nm) of a non-woven polystyrene fabric containing 1.
Figure S14. Photochemical stability experiment, i.e., UV-Vis absorption spectra of a toluene solution of 1 recorded after certain time intervals during the irradiation with white light.
2. Experimental Details

2.1 General information

The synthesis of 1 was performed under an inert atmosphere of dinitrogen by means of standard Schlenk-line techniques, while the samples for analytics were handled in a glovebox (GS Systemtechnik and MBraun). THF and toluene were dried using Na/benzophenone and distilled prior to use. Acetonitrile and dichloromethane were used as p.a. grade and distilled from calcium hydride and phosphorus pentoxide, respectively, while C₆D₆ was dried using molecular sieves (3 Å). Barium sulfate was dried at 250 °C prior to use. Polystyrene (PS, Mw = 350,000 g mol⁻¹) and trimethyl aluminium were purchased from Sigma-Aldrich (Germany). These chemicals were used as received. The protio-ligand (BODDI)H₂ was synthesized according to literature procedures.⁵¹

2.2 Characterization

The NMR spectra were recorded with Bruker Avance 400 spectrometer with δ referenced to external tetramethylsilane standard (¹H and ¹³C). ¹H and ¹³C NMR spectra were calibrated by using the solvent residual peak (C₆D₅H: δ(¹H) = 7.16 ppm) and the solvent peak (C₆D₆: δ(¹³C) = 128.06 ppm), respectively. Elemental analysis was performed with a Vario EL Cube (Elementar Analysensysteme GmbH). IR spectra (given in cm⁻¹) were recorded with an Agilent Cary 630 FT-IR spectrometer using a diamond ATR unit. (Uncorrected) melting points were determined with an Apotec capillary melting point apparatus.

2.3 Synthetic procedures

At 0 °C Trimethylaluminium (1.14 mL, 2.28 mmol, 2 M in toluene) was added to a solution of (BODDI)H₂ (500 mg, 1.09 mmol) in 3 mL of toluene and stirred overnight at room temperature. The suspension containing a yellow precipitate was heated up to 100 °C and slowly cooled to room temperature for crystallization. The yellow crystals were separated and dried in vacuum affording 480 mg, 0.84 mmol, 77 % yield.

¹H NMR (400 MHz, C₆D₆): δ [ppm] = -0.37 (s, 12 H, Al(CH₃)₂), 1.13 (d, J = 7.02 Hz, 12 H, CH(CH₃)₂), 1.30 (d, J=6.7 Hz, 12 H, CH(CH₃)₂), 1.49 (s, 6 H, α-CH₃), 3.24 (sept, J = 6.8 Hz, 4 H, CH(CH₃)₂), 5.07 (s, 2 H, β-CH), 7.04 - 7.13 (m, 6 H, ArH); ¹H NMR (400 MHz, toluene-d₈): δ = 7.04-7.12 (m, 6H, ArH), 4.98-5.00 (s, 2H, β-CH), 3.21 (sept, J = 6.9 Hz, 4H, CH(CH₃)₂), 1.49 (s, 6H, α-CH₃), 1.28 (d, J = 6.7 Hz, 12H, CH(CH₃)₂), 1.14 (d, J = 7.0 Hz, 12H, CH(CH₃)₂), -0.46 ppm (s, 12H, Al(CH₃)₂); ¹³C NMR (101 MHz,
2.4 Electrospinning

Solutions (5 mL) containing 10 % (w/w) of complex 1 with respect to polystyrene (PS) were prepared for electrospinning by dissolving 810 mg of PS in 4.1 g of THF and addition of 90 mg of 1. For comparison, a reference solution (free of 1) was prepared from 0.9 g of PS and 4.1 g of THF.

Electrospinning was carried out using a commercial air conditioned electrospinning machine E-Spintronic (Erich Huber GmbH, Germany) at 26 °C and air humidity of 33 %. The integrated infusion pump was mounted with a 5 ml plastic syringe connected with a 35 cm PTFE tube (Intra special catheters GmbH, Germany) to the nozzle of a stainless-steel straight-end hollow needle (0.4 mm). A grounded glass plate (25x25 cm²) was used as collector for collecting the electrospun fibers. The distance between the needle tip and the collector was maintained at 20 cm. The voltage applied to the needle was adjusted to 36 kV. The polymer solution was fed at a constant rate of 1.0 ml h⁻¹ to the needle tip. The integrated IR lamp was turned on for faster solvent evaporation. The spinning of 0.5 ml of polymer solution lead to electrospun non-woven fabrics of approximately 80 cm².

Please note that electrospinning with other polymers (polycaprolactone, polymethylmethacrylate) was attempted but remained without success.

2.5 Scanning electron microscopy

The fiber morphology has been examined using a field-emission scanning electron microscope (SEM) Supra 55VP (Carl Zeiss, Germany). Si-wafer were used as substrate material for the fibers and Au was sputtered on the specimens to ensure a sufficient electric conductivity for the analysis. The images were taken by the SE2-Detector using 5 keV of excitation energy.
2.6 Energy-dispersive X-ray spectroscopy

Energy dispersive X-ray spectroscopy (EDX) was performed using the SEM mentioned before equipped with an EDX-system (Quantax with Si(Li)-detector, Bruker Nano GmbH, Germany). The electrospun fibers on a silicon wafer were sputtered with carbon. For the measurements, an excitation energy of 2 keV was used. The EDX investigation shows only a small signal accounting for aluminium, Figure S10, which is in agreement with the low concentration, i.e., 10 % (w/w), of 1 in the polymer matrix and the hence low overall aluminium content. Thus, EDX mapping of the homogeneous distribution within the fibers could not be demonstrated.

2.7 Absorption and emission measurements

Absorption and diffuse reflectance spectra were recorded at a JASCO V780 UV-Visible/NIR spectrophotometer (JASCO GmbH, Pfungstadt, Germany). Absorption spectra in solution were recorded in a cell with 1 cm path length in toluene, dichloromethane and acetonitrile as solvent. In the diffuse reflectance measurements using an integrating sphere pure BaSO$_4$ powder or an electro-spun fiber mat (without embedded dye) served as reference. In case of the powder sample and the fiber mat we observed a local color change after the measurement. Hence, the bulk powder sample was illuminated for 24 hours using a 410 nm LED, affording a yellow powder. $^1$H NMR spectroscopy reveals the primary formation of the protio-ligand (BODDI)$_2$H$_2$ likely caused by hydrolysis in air.

Photoluminescence spectra were recorded using an FLS980 photoluminescence spectrometer (Edinburgh Instruments Ltd., Livingston, UK). An excitation wavelength of 410 nm was used. For luminescence spectra of the solution the optical density of the solutions was set to 0.05-0.10 to avoid inner filter effects and reabsorption of photoluminescence. Emission spectra of the solid samples were recorded using an integrating sphere. Absolute quantum yields were determined from the solution and the solid samples (solid and fiber mat) using an integrating sphere. Effects due to indirect excitation from scattered excitation light were corrected for in the measurement protocol for the powder samples. Further, the impact of reabsorption on the determined values for the powder samples was evaluated by diluting the samples with BaSO$_4$. Values determined by these procedure were additionally verified by relative quantum yield measurement using perylene as reference.
2.8 Fluorescence lifetime measurements

Photoluminescence decay curves were determined employing a Hamamatsu HPDTA streak camera (C4334, Hamamatsu Photonics K.K., Hamamatsu, Germany). Samples were excited by pulses centered at 390 nm created by frequency-doubling the output of a Ti:Sapphire laser (Tsunami, Newport Spectra-Physics GmbH, Berlin, Germany). The repetition rate of the fundamental is reduced to 400 kHz by a pulse selector (model 3980, Newport Spectra-Physics GmbH, Berlin, Germany). Photoluminescence was collected for solutions in oxygen free toluene in a 1 cm inert cuvette in a 90° angle and spectrally dispersed on the detector using a CHROMEX spectrograph (Chromex, Albuquerque, NM, USA), yielding a dataset in the spectral range of 410-550 nm and a maximum decay time of 10 ns. The optical density of the solutions was adjusted to circa 0.1 at the excitation wavelength. Measurements were performed with a polarizer set to magic angle, i.e., set to 54.7° with respect to the excitation polarization, in the detection path. A glass plate was used to record the instrumental response function (IRF) by reflecting parts of the attenuated excitation beam directly into the detector. IRFs were typically in the order of 0.25 ns. The emission was spectrally integrated and the resulting decay traces fitted with DecayFit software.

2.9 Cyclic voltammetry

Cyclic voltammetry was conducted in a nitrogen flushed glove box (MBraun, H₂O < 0.1 ppm, O₂ < 0.1 ppm) using a VersaStat3 potentiostat. Measurements were performed in a three-electrode electrochemical cell containing a glassy carbon working electrode (3 mm diameter), a platinated titanium wire counter electrode and a silver wire pseudoreference electrode. Prior to the measurement, glassy carbon electrodes were polished on felt polishing pads with aqueous suspensions of 0.3 µm and 0.05 µm alumina. The electrode was subsequently rinsed with de-ionized water and dried. Electrochemical cells were filled with 4 mL of the electrolyte, which was prepared from anhydrous and degassed MeCN and anhydrous tetrabutylammonium hexafluorophosphate (recrystallized from ethanol, 0.1 M). A sample concentration of about 0.2 mM was used. Ferrocene was added as internal reference before recording the last cyclic voltammogram.
**2.10 Fluorescence lifetime imaging**

FLIM experiments were performed on custom Abberior Expert Line laser scanning STED microscope with 100×/1.4 oil immersion objective lens from Olympus. Pulsed 440nm excitation laser repetition rate 40 MHz was used for the lifetime imaging with very low excitation power since the dye was extremely bright. Fluorescence was collected a 1.0 airy unit pinhole, and finally collected by single photon counting SPCM-AQRH-14-TR avalanche photodiodes (Excelitas Technologies) equipped with appropriate filters. For the fibermat and crystal lifetime measurements, the pixel size was 60 nm in all dimensions and pixel dwell time was 100 µs with 30 line accumulation. A few of the crystals were carefully extracted with tweezer and placed on the center of a plasma cleaned glass coverslip (#1.5) and then mounted on Attofluor chamber (Thermo Fisher Scientific) which was filled with argon gas and sealed with parafilm to minimize exposure to moisture. Then it was mounted on the microscope for imaging. For generation of fluorescence lifetime images of single molecules, the signal of the avalanche photodiode was fed into a time-correlated single-photon-counting (TCSPC) PCI card from Becker & Hickl, Berlin, Germany. SPCImage software (Becker & Hickl, Berlin, Germany) was used for fitting the lifetime data.
3. Crystallographic Details

The intensity data for the compound 1 were collected on a Nonius KappaCCD diffractometer using graphite-monochromated Mo-Kα radiation. Data were corrected for Lorentz and polarization effects; absorption was taken into account on a semi-empirical basis using multiple-scans[82-4]. The structure was solved by intrinsic phases (SHELXT [55]) and refined by full-matrix least squares techniques against Fo² (SHELXL-2018 [56]). All hydrogen atoms were included at calculated positions with fixed thermal parameters. All non-hydrogen atoms were refined anisotropically[56]. Olex2 [57] was used for structure representations.

Crystal Data for 1: C₃₅H₅₄Al₂N₂O, Mr = 572.76 g mol⁻¹, light-yellow prism, size 0.108 x 0.102 x 0.092 mm³, monoclinic, space group C 2/c, a = 16.3795(3), b = 9.0045(2), c = 24.3046(4) Å, β = 105.676(1)°, V = 3451.33(12) Å³, T= -140 °C, Z = 4, ρcalc. = 1.102 gcm⁻³, μ (Mo-Kα) = 1.12 cm⁻¹, multi-scan, transmin: 0.7119, transmax: 0.7456, F(000) = 1248, 12839 reflections in h(-21/21), k(-11/11), l(-31/26), measured in the range 2.583° ≤ Θ ≤ 27.469°, completeness Θmax = 99.9%, 3945 independent reflections, Rint = 0.0332, 3506 reflections with Fo > 4σ(Fo), 189 parameters, 0 restraints, R₁(obs) = 0.0420, wR²(obs) = 0.0966, R₁(all) = 0.0482, wR²(all) = 0.1006, GOOF = 1.055, largest difference peak and hole: 0.307 / -0.258 e Å⁻³.

Supporting Information available: Crystallographic data (excluding structure factors) has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication CCDC-2082119 for 1. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 1EZ, UK [E- mail: deposit@ccdc.cam.ac.uk].
4. Computational Details

All quantum chemical calculations determining structural and electronic properties of the present aluminium-based photosensitizer \textbf{1} were obtained by the Gaussian 16 program.\textsuperscript{58} The fully relaxed equilibrium geometry of \textbf{1} within the singlet ground state was obtained at the density functional level of theory (DFT) by means of the B3LYP\textsuperscript{59} XC functional (or B3LYP20) as well as utilizing a functional denoted B3LYP10 based on B3LYP, comprising 10 \% of exact-exchange, respectively, 58.5 \% of non-local B88\textsuperscript{10} exchange and the LYP\textsuperscript{9b} correlation. The def2-SVP basis\textsuperscript{11} set was applied for all atoms. A vibrational analysis was carried out to verify that a minimum on the 3N-6 dimensional potential-energy (hyper)surface (PES) was obtained within the B3LYP as well as within the B3LYP10 equilibrium structures.

Subsequently, excited state properties such as excitation energies, oscillator strengths and electronic characters were calculated within the Franck-Condon structure at the time-dependent DFT (TDDFT) level of theory. Therefore, the 50 lowest singlet excited states were calculated within the B3LYP as well as within B3LYP10 equilibrium structure. Thereby, the same XC functional and basis set was applied as for the preceding ground state calculation, respectively. Several joint spectroscopic-theoretical studies successfully applied TDDFT, \textit{i.e.} the B3LYP functional, to investigate excited state properties in the scope of UV-Vis spectroscopy, for Al(III)-based coordination compounds.\textsuperscript{512} Effects of interaction with a solvent (toluene: $\varepsilon = 2.374$, $n = 1.497$) were taken into account on the ground and excited states properties by the solute electron density (SMD) variant of the integral equation formalism of the polarizable continuum model.\textsuperscript{513} The non-equilibrium procedure of solvation was used for the calculation of the excitation energies within the Franck-Condon point, which is well adapted for processes where only the fast reorganization of the electronic distribution of the solvent is important. All calculations were performed including D3 dispersion correction with Becke-Johnson damping.\textsuperscript{514}

Furthermore, excited state relaxation pathways accessible upon excitation into the lowest singlet excited state within the Franck-Condon point were elucidated by TDDFT. Therefore, fully relaxed equilibrium structures were obtained exclusively at the B3LYP10/def2-SVP level of theory for the $S_1$ and $S_2$ Franck-Condon states of $\pi\pi^*$ and $\sigma\pi^*$ nature, respectively. In case of (excited state) optimizations, the equilibrium procedure of solvation was applied to account for state-specific solvent relaxation (toluene).
Figure S15. Simulated electronic absorption spectrum of 1 obtained at the TD-DFT level of theory, i.e. using the B3LYP20 (solid, grey) vs. the B3LYP10 (solid black) XC functional. The calculated emission spectrum, as obtained at the B3LYP10 level of theory within the fully relaxed equilibrium S1 state of ππ* character, is shown in dashed (black). All simulations include D3BJ dispersion correction and solvent effects (toluene) by a polarizable continuum model. Charge density differences (CDDs) visualize the electronic nature of the respective transitions; charge transfer takes place from red to blue.

Table S1. Excited state properties, such as electronic character, excitation energy, wavelength, and oscillator strength, of the singlet excitations contributing to the UV/vis absorption of 1 obtained at the TDDFT level of theory (B3LYP20/def2-svp and B3LYP10/def2-svp) including D3BJ dispersion correction and solvent effects (toluene) by a polarizable continuum model.

| State | Transition | Weight (%) | ΔE° (eV) | λ (nm) | f | λexp (nm) |
|-------|------------|------------|-----------|--------|---|-----------|
| B3LYP20 | π(156) → π*(157) | 98 | 3.30 | 376 | 0.8045 | 455 |
| | σ(155) → π*(157) | 99 | 3.84 | 323 | 0.0010 | - |
| | π(154) → π*(157) | 95 | 3.96 | 313 | 0.0195 | - |
| | σ(153) → π*(157) | 78 | 3.97 | 312 | 0.0024 | - |
| | π(151) → π*(157) | 20 | | | | |
| B3LYP10 | π(156) → π*(157) | 98 | 3.09 | 402 | 0.9252 | 455 |
| | σ(155) → π*(157) | 97 | 3.52 | 353 | 0.0017 | - |
| | σ(153) → π*(157) | 97 | 3.65 | 340 | 0.0020 | - |
| | π(154) → π*(157) | 98 | 3.65 | 340 | 0.0373 | - |
Table S2. Molecular orbitals involved in the Franck-Condon electronic transitions of interest (recall Table S1) of 1 obtained at the TDDFT level of theory (B3LYP20/def2-svp and B3LYP10/def2-svp) including D3BJ dispersion correction and solvent effects (toluene) by a polarizable continuum model.

| B3LYP20 (FC) |
|--------------|
| ![Molecular orbitals](image1) | ![Molecular orbitals](image2) | ![Molecular orbitals](image3) | ![Molecular orbitals](image4) |
| $\sigma(151)$ | $\sigma(152)$ | $\sigma(153)$ | $\sigma(154)$ |
| $\sigma(155)$ | $\pi(156)$ | $\pi^*(157)$ |

| B3LYP10 (FC) |
|--------------|
| ![Molecular orbitals](image5) | ![Molecular orbitals](image6) | ![Molecular orbitals](image7) | ![Molecular orbitals](image8) |
| $\sigma(153)$ | $\pi(154)$ | $\sigma(155)$ | $\pi(156)$ |
| $\pi^*(157)$ |
Table S3. Charge density differences (CDDs) visualizing the nature of the Franck-Condon electronic transitions of interest (recall Table S1) of 1 obtained at the TDDFT level of theory (B3LYP20/def2-svp and B3LYP10/def2-svp) including D3BJ dispersion correction and solvent effects (toluene) by a polarizable continuum model. Charge transfer occurs from red to blue.

| B3LYP20 (FC) |
|--------------|
| $S_1(\pi\pi^*)$ | $S_2(\sigma\pi^*)$ | $S_3(\pi\pi^*)$ | $S_4(\sigma\pi^*)$ |

| B3LYP10 (FC) |
|--------------|
| $S_1(\pi\pi^*)$ | $S_2(\sigma\pi^*)$ | $S_3(\sigma\pi^*)$ | $S_4(\pi\pi^*)$ |

Table S4. Charge density differences (CDDs) visualizing the nature of the electronic transitions of interest of 1 within the fully relaxed excited singlet state structures $S_1(\pi\pi^*)$ and $S_2(\sigma\pi^*)$; labels are given for FC structure. Results were obtained at the TDDFT level of theory (B3LYP10/def2-svp) including D3BJ dispersion correction and solvent effects (toluene) by a polarizable continuum model. Charge transfer occurs from red to blue.

| B3LYP10 ($\pi\pi^*$) |
|----------------------|
| $S_1(\pi\pi^*)$ | $S_2(\sigma\pi^*)$ | $S_3(\pi\pi^*)$ | $S_4(\sigma\pi^*)$ |

| B3LYP10 ($\sigma\pi^*$) |
|----------------------|
| $S_1(\sigma\pi^*)$ | $S_2(\sigma\pi^*)$ | $S_3(\pi\pi^*)$ | $S_4(\pi\pi^*)$ |
Table S5. Relevant structural parameter involved in the light-induced excited state relaxation pathways of 1, i.e., Al–CH₃ bond lengths ($r_1$, $r_1'$, $r_2$ and $r_2'$).

| Equilibrium structure | $r_1$ (Å) | $r_2$ (Å) | $r_1'$ (Å) | $r_2'$ (Å) |
|------------------------|-----------|-----------|------------|------------|
| FC                     | 1.9625    | 1.9677    | 1.9625     | 1.9677     |
| $\pi\pi^*$             | 1.9629    | 1.9699    | 1.9629     | 1.9699     |
| $\sigma\pi^*$          | 1.9527    | 2.1903    | 1.9706     | 1.9746     |
5. NMR and IR spectra

Figure S16. $^1$H NMR spectrum (400 MHz) of 1 in C$_6$D$_6$.

Figure S17. $^{13}$C NMR spectrum (101 MHz) of 1 in C$_6$D$_6$. 
Figure S18. $^1$H NMR spectrum (400 MHz) of 1 in toluene-d$_8$.

Figure S19. $^{13}$C NMR spectrum (101 MHz) of 1 in toluene-d$_8$. 
Figure S20. $^{27}\text{Al}$ NMR spectrum (104 MHz) of 1 in $\text{C}_6\text{D}_6$. The signal at 76 ppm accounts for the background/probe.

Figure S21. $^1\text{H}$ NMR spectrum (400 MHz) of 1 in CDCl$_3$. 
Figure S22. $^1$H NMR spectrum (400 MHz) of 1 in CDCl$_3$ after heating to 60°C for 4 h.

Figure S23. $^1$H NMR spectrum (400 MHz) of 1 in CDCl$_3$ after heating to 60°C for 3 days.
Figure S24. $^1$H NMR spectrum (400 MHz) of 1 in THF-d$_8$.

Figure S25. $^1$H NMR spectrum (400 MHz) of 1 in THF-d$_8$ after heating to 60°C for 4 h.
Figure S26. $^1$H NMR spectrum (400 MHz) of 1 in THF-d$_8$ after heating to 60°C for 3 days

Figure S27. ATR-IR (diamond) spectrum of 1.
### Franck-Condon structure (S6)

#### B3LYP/def2svp

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 2.114021 | -0.597492 | 0.532274 |
| C    | 1.768653 | -0.628737 | 0.532274 |
| H    | 2.446057 | -0.597492 | 0.532274 |
| C    | 2.895800 | -0.628737 | 0.532274 |
| C    | 3.037619 | -0.597492 | 0.532274 |
| H    | 3.435301 | -0.628737 | 0.532274 |
| C    | 4.038776 | -0.597492 | 0.532274 |
| C    | 4.154541 | -0.628737 | 0.532274 |
| N    | 4.560785 | -0.597492 | 0.532274 |

### Franck-Condon structure (S10)

#### B3LYP/def2svp

| Atom | X       | Y       | Z       |
|------|---------|---------|---------|
| C    | 2.114021 | -0.597492 | 0.532274 |
| C    | 1.768653 | -0.628737 | 0.532274 |
| H    | 2.446057 | -0.597492 | 0.532274 |
| C    | 2.895800 | -0.628737 | 0.532274 |
| C    | 3.037619 | -0.597492 | 0.532274 |
| H    | 3.435301 | -0.628737 | 0.532274 |
| C    | 4.038776 | -0.597492 | 0.532274 |
| C    | 4.154541 | -0.628737 | 0.532274 |
| N    | 4.560785 | -0.597492 | 0.532274 |
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