Supporting Information

High-Throughput Single-Molecule Spectroscopy Resolves the Conformational Isomers of BODIPY Chromophores

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Experimental Procedures

Materials and Methods. Chemicals were purchased from commercial sources and used as received. CH_2Cl_2 and MeCN were distilled over CaH_2. Tetrahydrofuran (THF) was distilled over Na and benzophenone. H_2O (18.2 MΩ cm) was purified with a Barnstead International NANOpure Diamond analytical system. Compounds **3**, **4** and **8** were prepared according to a literature procedure.[S1,S2] Electrospray ionization mass spectra (ESIMS) were recorded with a Bruker micrOTO-Q II spectrometer. Nuclear magnetic resonance (NMR) spectra were recorded with Bruker 300, 400 and 500 spectrometers. Absorption spectra were recorded with a Varian Cary 100 Bio spectrometer in quartz cells with path length of 1.0 cm. Emission and excitation spectra were recorded with a Varian Cary Eclipse spectrometer in aerated solutions. Fluorescence quantum yields were determined against a solution of **8** (ϕ = 0.50)[S2] in MeCN, following a literature protocol.[S3]

1. *N*-Bromosuccinimide (NBS, 1.34 g, 7.5 mmol) and azobis-*iso*-butyrronitrile (AIBN, 62.4 mg, 0.4 mmol) were added to a solution of 2-methylbenzoxazole (1.00 g, 7.5 mmol) in CCl_4 (10 mL) stirred at ambient temperature under Ar. The reaction mixture was warmed up to 70 °C and stirred at this temperature for 19 hours. The resulting suspension was cooled down to ambient temperature and filtered. The solvent of the filtrate was distilled off under reduced pressure and the residue was purified by column chromatography [SiO_2, hexane/CH_2Cl_2/EtOAc (30:10:1, v/v/v)] to afford **1** (0.65 g, 41%). ESIMS: *m/z* calcd for $C_8H_6BrNNaO^+$ = 234.0; *m/z* found = 234.0 $[M + Na]^+$; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.77–7.74 (m, 1H), 7.60–7.54 (m, 1H), 7.45–7.35 (m, 2H), 4.62 (s, 2H).

2. A suspension of **1** (0.63 g, 3.0 mmol) in $P(OEt)_3$ (1.02 mL, 5.98 mmol) was heated under reflux for 2 hours. After cooling down to ambient temperature, the mixture was diluted with EtOAc (5 mL) and washed with aqueous HCl (1 M, 3 × 10 mL). The organic phase was dried over Na_2SO_4 and the solved was distilled off under reduced pressure. The residue was purified by column chromatography [SiO_2, CH_2Cl_2/EtOAc (50:50, v/v)] to afford **2** (0.29 g, 36%) as clear liquid. ESIMS: *m/z* calcd for $C_{12}H_{16}NO_4P$ = 269.0817; *m/z* found = 270.0899 $[M + H]^+$; ^1H NMR (300 MHz, $CDCl_3$): δ = 7.73–7.69 (m, 1H), 7.58–7.52 (m, 1H), 7.39–7.32 (m, 2H), 4.27–4.16 (m, 4H), 3.63 (s, 1H), 3.56 (s, 1H), 1.35 (m, 6H).

BO. A solution of *n*-Buli (0.41 mmol, 2.5 M) in hexane (0.16 mL) was added dropwise to a solution of **2** (100 mg, 0.37 mmol) in THF (5 mL) stirred at –78 °C under Ar. After 15 minutes of stirring at this temperature, a solution of **3** (0.15 g, 0.37 mmol) in THF (3 mL) was added dropwise and the mixture was allowed to warm up to ambient temperature with stirring and maintained under these conditions for a further 15 hours. The solvent was distilled off under reduced pressure and the residue was dissolved in EtOAc (15 mL) and washed with a saturated aqueous solution of NaCl (3 × 20 mL). The organic phase was dried over Na_2SO_4 and the solved was distilled off under reduced pressure. The residue was purified by column chromatography [SiO_2, hexane/ CH_2Cl_2/EtOAc (80:15:5, v/v) → $CHCl_3$/hexane (50:10, v/v)] to afford **BO** (40 mg, 21%) as a dark gold solid. ESIMS: *m/z* calcd for $C_{31}H_{30}BF_2N_3O$ = 509.2450; *m/z* found = 510.2529 $[M + H]^+$; ^1H NMR (300 MHz,

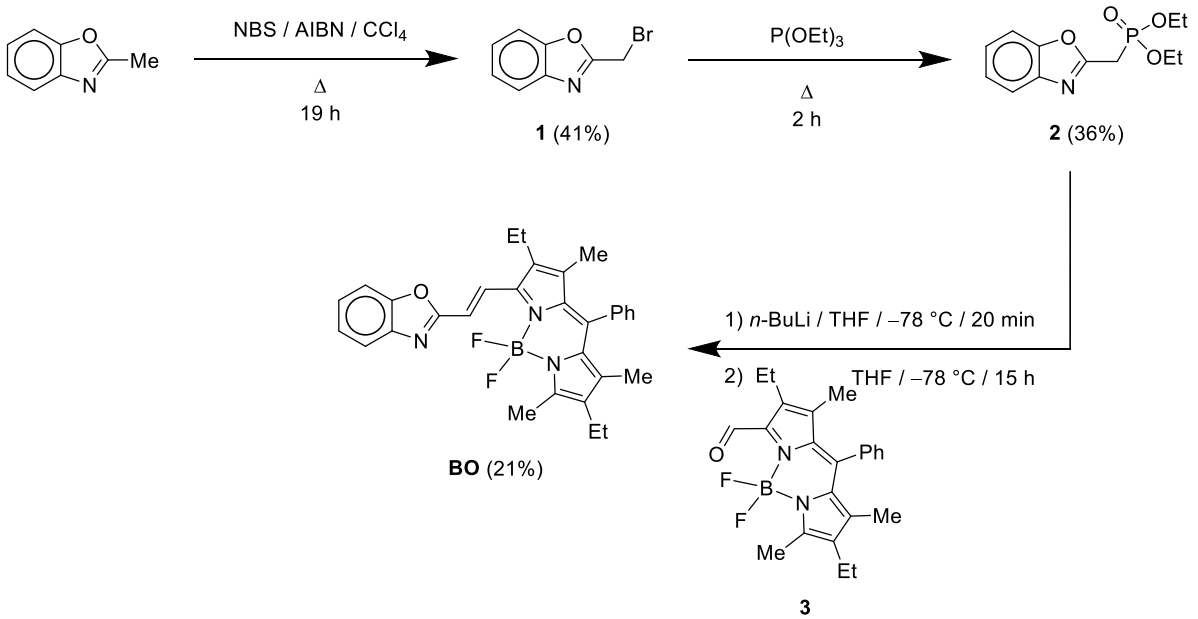

Figure S1. Synthesis of **BO**.

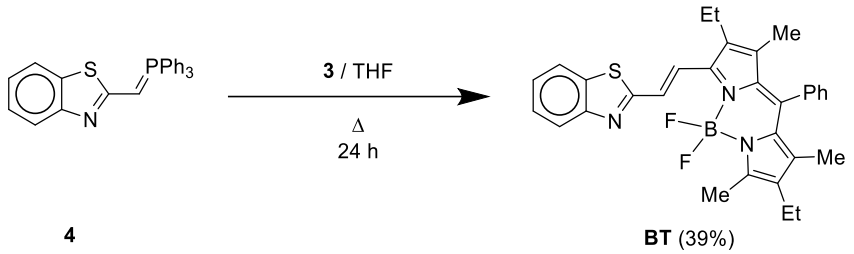

Figure S2. Synthesis of **BT**.

$CDCl_3$): δ = 8.29 (d, 16.7 Hz, 1H), 7.78–7.66 (m, 1H), 7.60 (dd, 6.8 and 2.3 Hz, 1H), 7.57–7.46 (m, 3H), 7.44–7.29 (m, 4H), 7.17 (d, 16.7 Hz, 1H), 2.77–2.54 (m, 5H), 2.35 (q, 7.5 Hz, 2H), 1.33 (m, 6H), 1.17 (t, 7.5 Hz, 3H), 1.02 (t, 7.5 Hz, 3H).

BT. A solution of **3** (50 mg, 0.13 mmol) and **4** (121 mg, 0.29 mmol) in THF (25 mL) was stirred under reflux and Ar for 24 hours. After cooling down to ambient temperature, the solvent was distilled off under reduced pressure and the residue was purified by column chromatography [SiO_2, CH_2Cl_2] to afford **BT** (27 mg, 39%) as a gold solid. ESIMS: *m/z* calcd for $C_{31}H_{30}BF_2N_3S$ = 525.2222; *m/z* found = 526.2302 $[M + H]^+$; ^1H NMR (400 MHz, $CDCl_3$): δ = 8.07 (d, 16.8 Hz, 1H), 8.01 (d, 8.1 Hz, 1H), 7.87 (d, 7.9 Hz, 1H), 7.60–7.43 (m, 5H), 7.43–7.29 (m, 3H), 2.74–2.56 (m, 5H), 2.35 (q, 7.7 Hz, 2H), 1.39–1.29 (m, 6H), 1.17 (t, 7.6 Hz, 3H), 1.02 (t, 7.6 Hz, 3H).

5. NBS (1.83 g, 10.31 mmol) and AIBN (169 mg, 1.03 mmol) were added to a solution of 2-methyl-5-nitrobenzothiazole (2 g, 10.31 mmol) in CCl_4 (20 mL) stirred at ambient temperature under Ar. The reaction mixture was warmed up to 70 °C and stirred at this temperature for 5 hours. The resulting suspension was cooled down to ambient temperature and filtered. The solvent of the filtrate was distilled off under reduced pressure and the residue was purified by column chromatography [SiO_2, hexane/ EtOAc (60:10 v/v)] to afford **5** (0.42 g, 15 %). ^1H NMR (300 MHz, $CDCl_3$) δ = 8.85 (d, 2.2 Hz, 1H), 8.49–8.32 (m, 1H), 8.14 (dd, 9.1 and 1.2 Hz, 1H), 4.86 (s, 2H).

6. A solution of **5** (0.38 g, 1.40 mmol) and PPh_3 (0.47 g, 1.68 mmol) in PhMe (7 mL) was heated under reflux for 24 hours. After cooling down to ambient temperature, the mixture was filtered and the solid residue was dried under vacuum to afford **6** (0.41 g, 60 %) as a sticky solid. ^1H NMR (300 MHz, DMSO-d_6) δ = 9.19–9.11 (m, 1H), 8.34–7.48 (m, 1H), 8.06–7.99 (m, 1H), 7.95–7.48 (m, 15H), 6.17 (d, 15.8 Hz, 2H).

7. *t*-BuOK (130 mg, 1.16 mmol) was added to a solution of **6** (400 mg, 0.75 mmol) in PhMe (5 mL) stirred at ambient temperature under Ar. The mixture was stirred under these conditions for 14 hours and filtered. The solvent of the filtrate was distilled off under reduced pressure and the residue was dissolved in the minimum amount of CH_2Cl_2. Hexane was gradually added to obtain a turbid solution, which was stored in the freezer overnight. The resulting red crystals were filtered

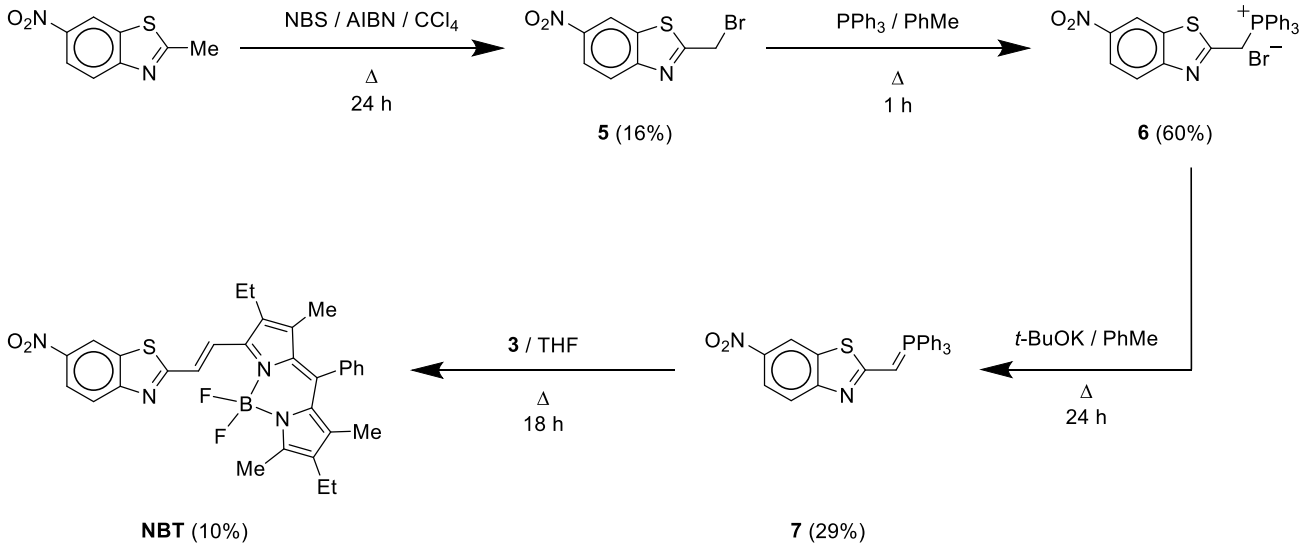

Figure S3. Synthesis of **NBT**.

off and dried to afford **7** (100 mg, 29 %). ^{1}H NMR (300 MHz, DMSO-d_6): δ = 8.37 (m, 1H), 7.87 (m, 1H), 7.80–7.51 (m, 16H), 6.89 (d, 9.2 Hz, 1H).

NBT. A solution of **3** (50 mg, 0.13 mmol) and **7** (90 mg, 0.19 mmol) in THF (5 mL) was heated under reflux for 18 hours. After cooling down to ambient temperature, the solvent was distilled off under reduced pressure and the reside was purified by column chromatography [SiO_2, hexane/EtOAc/CH_2Cl_2 (80:10:10, v/v/v)] to afford **NBT** (7.5 mg, 10%) as a yellow solid. ESIMS: *m/z* calcd for $C_{31}H_{29}BF_2N_4O_2S$ = 570.2072; *m/z* found: 571.2140 $[M + H]^+$; ^{1}H NMR (500 MHz, $CDCl_3$) δ = 8.79 (d, 2.4 Hz, 1H), 8.36 (dd, 9.0 and 2.3 Hz, 1H), 8.18 (d, 16.7 Hz, 1H), 8.07 (d, 9.0 Hz, 1H), 7.73–7.65 (m, 1H), 7.56–7.52 (m, 3H), 7.36–7.30 (m, 2H), 2.72–2.60 (m, 5H), 2.37 (q, 7.4 Hz, 2H), 1.35 (s, 3H), 1.34 (s, 3H), 1.18 (t, 7.5 Hz, 3H), 1.04 (t, 7.5 Hz, 3H).

Crystallographic Analysis. Single crystals of **BT**, suitable for diffraction analysis, grew from a CH_2Cl_2 solution of the compound maintained at ambient temperature, after diffusion of pentane vapors. The data crystal was mounted onto the end of a thin glass fiber using Paratone-N for data collection at 100 K under N_2. X-ray intensity data were measured by using a Bruker SMART APEX2 CCD-based diffractometer using Mo Kα radiation (λ = 0.71073 Å).[S4] The raw data frames were integrated with the SAINT+ program by using a narrow-frame integration algorithm.[S4] Corrections for Lorentz and polarization effects were also applied with SAINT+. An empirical absorption correction based on the multiple measurement of equivalent reflections was applied using the program SADABS. The structure was solved by a combination of direct methods and difference Fourier syntheses and refined by full-matrix least-squares on F_2, using the SHELXTL software package.[S5,S6] All non-hydrogen atoms were refined with anisotropic displacement parameters. Hydrogen atoms were placed in geometrically-idealized positions and included, as standard riding atoms, during the least-squares refinements. Crystal data, data collection parameters and results of the analyses are listed in Table S1. Compound **BT** crystallized in the monoclinic crystal system. The systematic absences in the intensity data identified the unique space group $P2_1/n$.

Computational Methods. Density-functional theory[S7] (DFT) calculations were performed with the 6-311+G(d,p) basis set and the restricted B3LYP[S8,S9] and M06HF[S10,S11] functionals implemented in Gaussian 09.[S12] Geometry optimizations and frequency calculations were carried out with the polarizable continuum model (PCM) for acetonitrile, using the integral equation formalism (IEF) variant.[S13] Molecular orbitals were computed at the same level of theory, including the solvation model. Single-point second-order Møller–Plesset perturbation (MP2) theory[S14] calculations were performed on the optimized geometries with the same basis set and solvation model. Time-dependent[S15] (TD) DFT calculations were performed with the same basis set, functionals and solvation model of the ground-state calculations.

Single-Molecule Spectroscopy. The optical setup for single-molecule imaging and spectroscopy was adapted from a literature precedent.[S16] Specifically, a continuous-wave laser was used for excitation (532 nm, 200 mW; Spectra Physics). The laser beam was guided into an inverted microscope (Nikon Ti-E) and subsequently focused by a lens (focal length = 400 mm) into the back focal plane of a total internal reflection (TIRF) objective (Nikon CFI Apochromat 100×, numerical aperture = 1.49). The collected fluorescence image was transmitted into a spectrometer, which consists of a transmission-type diffraction grating (100 grooves mm^{-1}, Panton Hawskely Education Ltd. STAR100) and two relay lenses (focal length = 50 mm). The image was split into a non-dispersed spatial image and a dispersed first-order spectral image at the grating. The distinguished spatial and spectral images were then captured by an electron-multiplying charge-coupled (EMCCD) camera (Andor iXon 897) simultaneously. A neutral density filter was inserted in the excitation beam line to adjust the beam power. Single-molecule imaging was performed using TIRF illumination with the excitation intensity of ~ 200 W cm^{-2} and the exposure time of 30 ms.

The time-dependent measurements for single-molecule spectral trajectory and fluctuation are acquired with the entrance slit width of 5 mm (wide-slit configuration) and concentrations of 10 pM with only a few sparse molecules in the entire field of view as illustrated in Figure 3***a***. For high-throughput SMS, we increase the concentration of compounds to 1 nM. The presence of single molecules is confirmed by the observations of single-step photobleaching as shown in Figure 3, as well as the narrow full width at half maximum of the point spread function of the diffraction-limited spot (less than 310 nm with our setup). As can be seen in the raw images (***a*** in Figure S18), there are significant overlapping between different single-molecule spectra using the wide-slit configuration. To achieve optimal spectral precision[S17] and minimize the possibility to detect overlapped single-molecule spectra, we adjust the entrance slit width to 50 μm (narrow-slit configuration, ***b*** in Figure S18) for high-throughput SMS. Under this condition, we collected ~10^4 molecules of each compounds within a few minutes by scanning of the microscope stage laterally. With wide-slit setup and low molecular concentration, SMS can also be still achieved with relatively low speed with scanning larger area of the substrates and results are consistent.

Sample Preparation for Single-Molecule Spectroscopy. Toluene solutions of **BO**, **BT** and **NBT** (10 pM for the acquisition of single-molecule spectra over time, 1 nM for high-throughput SMS) were spin-coated on No. 1 cover glasses with a Laurell

WS-650SZ-23NPPB spin coater operating at 2,000 rpm for 60 s. Prior to spin coating the cover glasses were cleaned with a South Bay Technology PC 2000 Plasma Cleaner. The microscope stage was scanned manually to *ca.* 10000 μm2 of the coated glass slides to ensure enough sampling. The single-molecule spectra were calibrated using their spatial locations as references and the overlapped spectra were removed using Matlab as detailed below.

Calibration Procedure. First, we acquired a calibration image, which is confined by a narrow slit, using a fluorescence calibration source. By integrating the acquired spectral image along the y-axis, we visualized the multiple emission peaks of the calibration source, centered at 487.7, 546.5, 611.6 and 707.0 nm (***a*** in Figure S4). Then, we obtained the calibration curve by fitting a relationship of the pixel positions and wavelengths of these emission peaks with a linear polynomial function (***b*** in Figure S4). We used the calibration curve to determine the nm/pixel ratio and the pixel shifts between the spatial and spectral images and calibrated emission spectra of single molecules by considering their spatial location and the corresponding pixel shifts.[S17] Lastly, the obtained spectra were further interpolated to each wavelength unit from 500–700 nm.

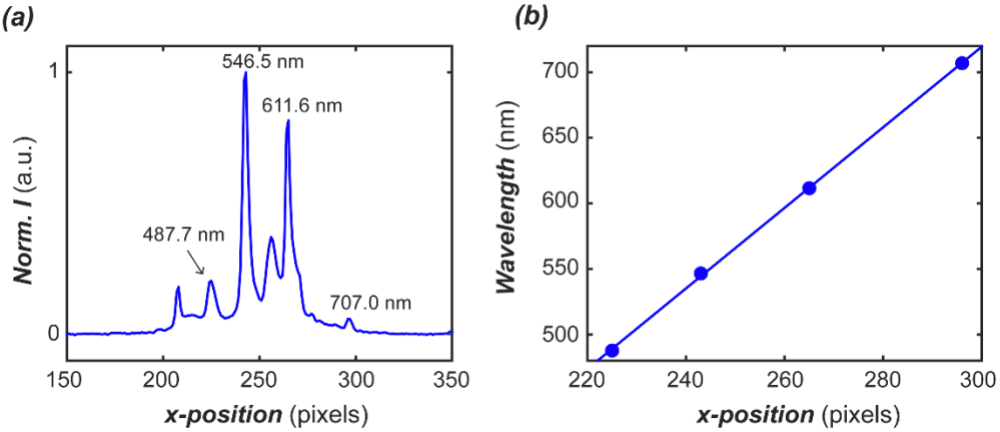

Figure S4. (***a***) Fluorescence lamp spectrum measured using the single-molecule spectroscopy system. (***b***) Calibration curve as a function between wavelength and pixel information on the EMCCD camera.

Spectral Centroid Calculation. The spectral centroid (SC) is calculated as the intensity-weighted average wavelength of every single-molecule spectra collecting from a spectral range of 500–700 nm using the equation below:

$$\mathrm{SC} = \sum_{n=500}^{n=700} I(n)W(n) / \sum_{n=500}^{n=700} W(n)$$

where $I(n)$ represents the intensity value at each wavelength after interpolation and $W(n)$ represents the wavelength.

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Table S1. Crystallographic Data for **BT**.

Empirical Formula	$C_{31}H_{30}BF_2N_3S$
Formula Weight	525.45
Crystal System	Monoclinic
Lattice Parameters	
a (Å)	10.8426(5)
b (Å)	21.9098(11)
c (Å)	11.8473(6)
β (deg)	106.849(1)
V (Å$_3$)	2693.6(2)
Space Group	$P2_1/n$ (#14)
Z Value	4
ρ_{calc} (g cm^{-3})	1.296
μ (Mo Kα) (mm^{-1})	0.160
Temperature (K)	100
$2\Theta_{max}$ (°)	50.00
No. Obs. [I > 2σ(I)]	3899
No. Parameters	348
Goodness of Fit	1.024
Max. Shift in Cycle	0.003
Residuals*: R1; wR2	0.0402; 0.0872
Absorption Correction, Max / Min	Multi-Scan 0.7457 / 0.6500
Largest Peak in Final Diff. Map (e Å^{-3})	0.344

*$R1 = \Sigma_{hkl}(\,||F_{obs}|-|F_{calc}||\,)/\Sigma_{hkl}|F_{obs}|$; $wR2 = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/\Sigma_{hkl}wF_{obs2}]^{1/2}$, $w = 1/\sigma^2(F_{obs})$; $GOF = [\Sigma_{hkl}w(|F_{obs}|-|F_{calc}|)^2/(n_{data} - n_{vari})]^{1/2}$.

Computational Data

*Coordinates of the geometry of isomer **ctt** of* **BT** *optimized with the B3LYP functional*

S	–4.957389000	1.761039000	0.224288000
F	–0.252736000	1.573714000	1.095006000
F	–0.335991000	1.582222000	–1.203942000
N	–4.973220000	–0.820595000	–0.176301000
N	0.433068000	–0.438485000	–0.087722000
N	1.827732000	1.643775000	–0.131584000
B	0.383394000	1.104213000	–0.084284000
C	–6.504522000	0.963854000	0.066721000
C	–7.789199000	1.506825000	0.122746000
H	–7.942406000	2.566815000	0.283812000
C	–8.870985000	0.647086000	–0.034621000
H	–9.877758000	1.046106000	0.004974000
C	–8.676363000	–0.729709000	–0.244297000
H	–9.537793000	–1.376380000	–0.363914000
C	–7.400138000	–1.270410000	–0.300161000
H	–7.243198000	–2.330405000	–0.461172000
C	–6.291930000	–0.422000000	–0.143580000
C	–4.158030000	0.182206000	–0.001837000
C	–2.711411000	0.130062000	0.025294000
H	–2.201610000	1.069899000	0.168635000
C	–2.032114000	–1.035005000	–0.106184000
H	–2.641191000	–1.924852000	–0.218024000
C	–0.620368000	–1.317202000	–0.102592000
C	–0.110745000	–2.645535000	–0.108883000
C	–0.936244000	–3.904498000	–0.107874000
H	–0.374923000	–4.700810000	–0.602826000
H	–1.834356000	–3.762257000	–0.714998000
C	–1.344935000	–4.375004000	1.300326000
H	–0.465458000	–4.571228000	1.919435000
H	–1.932009000	–5.295688000	1.243030000
H	–1.948984000	–3.618997000	1.808985000
C	1.281849000	–2.566486000	–0.077896000
C	2.200664000	–3.752836000	–0.049235000
H	1.627173000	–4.671536000	0.071749000
H	2.914789000	–3.696079000	0.773305000
H	2.781158000	–3.841425000	–0.970673000
C	1.615022000	–1.177086000	–0.078859000
C	2.879161000	–0.535931000	–0.093156000
C	4.126651000	–1.359763000	–0.082492000
C	4.684054000	–1.815179000	–1.281418000
H	4.203686000	–1.574071000	–2.223071000
C	5.854338000	–2.572360000	–1.269623000
H	6.279312000	–2.918589000	–2.204904000
C	6.475596000	–2.883280000	–0.060112000
H	7.384754000	–3.473588000	–0.051399000
C	5.922563000	–2.431729000	1.138118000
H	6.400250000	–2.669079000	2.081878000
C	4.754112000	–1.671661000	1.127691000
H	4.327076000	–1.320842000	2.060513000
C	2.983017000	0.852725000	–0.124569000
C	4.116616000	1.740661000	–0.172332000
C	5.572750000	1.389674000	–0.184048000

H	6.177833000	2.289496000	–0.296929000
H	5.821245000	0.708955000	–1.000506000
H	5.875827000	0.897547000	0.743316000
C	3.609432000	3.035740000	–0.210803000
C	4.381379000	4.326378000	–0.256445000
H	3.785783000	5.086177000	–0.770464000
H	5.280560000	4.191982000	–0.864336000
C	4.784823000	4.853250000	1.133222000
H	3.905775000	5.035145000	1.757551000
H	5.336622000	5.793046000	1.044095000
H	5.421342000	4.134201000	1.655571000
C	2.191997000	2.938910000	–0.180350000
C	1.219870000	4.069407000	–0.230486000
H	0.264574000	3.800455000	0.215139000
H	1.035979000	4.365101000	–1.269546000
H	1.621243000	4.940293000	0.289670000

Coordinates of the geometry of isomer ***ctc*** *of* **BT** *optimized with the B3LYP functional*

S	–5.201209000	–1.331006000	–0.146868000
F	–0.306944000	1.547662000	1.086569000
F	–0.362455000	1.569939000	–1.213496000
N	–4.810806000	1.248496000	0.044826000
N	0.443246000	–0.438067000	–0.098505000
N	1.785434000	1.679435000	–0.116061000
B	0.354471000	1.103272000	–0.086864000
C	–6.602874000	–0.285124000	–0.074345000
C	–7.955767000	–0.623969000	–0.102374000
H	–8.274426000	–1.656283000	–0.178288000
C	–8.889321000	0.405607000	–0.029728000
H	–9.946173000	0.166591000	–0.049550000
C	–8.482185000	1.747196000	0.068237000
H	–9.231347000	2.528358000	0.122640000
C	–7.136148000	2.083589000	0.096281000
H	–6.813564000	3.115252000	0.172139000
C	–6.177153000	1.061208000	0.025291000
C	–4.159941000	0.118991000	–0.035041000
C	–2.717128000	0.051780000	–0.030491000
H	–2.239288000	1.016233000	0.048273000
C	–2.006249000	–1.098451000	–0.106831000
H	–2.574807000	–2.020667000	–0.169189000
C	–0.586771000	–1.343831000	–0.106770000
C	–0.043375000	–2.658483000	–0.109344000
C	–0.833850000	–3.939999000	–0.101373000
H	–0.257036000	–4.718796000	–0.606202000
H	–1.742991000	–3.823134000	–0.697439000
C	–1.209965000	–4.426135000	1.310571000
H	–0.316828000	–4.600655000	1.916434000
H	–1.772572000	–5.362222000	1.257978000
H	–1.826736000	–3.688741000	1.831203000
C	1.347073000	–2.543169000	–0.085527000
C	2.296450000	–3.705259000	–0.060000000
H	1.747043000	–4.639347000	0.054736000
H	3.006618000	–3.634156000	0.764945000
H	2.881760000	–3.773568000	–0.980021000
C	1.643698000	–1.146126000	–0.089578000

C	2.891463000	–0.472830000	–0.096500000
C	4.159135000	–1.265126000	–0.090746000
C	4.726152000	–1.700519000	–1.292605000
H	4.238452000	–1.467273000	–2.232473000
C	5.915211000	–2.427951000	–1.285881000
H	6.347685000	–2.758670000	–2.223321000
C	6.545425000	–2.729250000	–0.078568000
H	7.469087000	–3.296634000	–0.073788000
C	5.982582000	–2.297991000	1.122547000
H	6.467124000	–2.528238000	2.064566000
C	4.795572000	–1.567194000	1.117229000
H	4.360931000	–1.231988000	2.052264000
C	2.960385000	0.917768000	–0.114081000
C	4.071622000	1.834510000	–0.149356000
C	5.536093000	1.520272000	–0.159373000
H	6.118279000	2.435121000	–0.271836000
H	5.802714000	0.845338000	–0.974763000
H	5.850247000	1.036843000	0.768962000
C	3.532074000	3.116458000	–0.175369000
C	4.270540000	4.426922000	–0.203990000
H	3.657743000	5.176352000	–0.712957000
H	5.175722000	4.322243000	–0.808841000
C	4.654070000	4.949335000	1.192961000
H	3.768045000	5.101941000	1.815271000
H	5.181733000	5.903960000	1.116172000
H	5.306752000	4.241522000	1.710668000
C	2.117106000	2.983487000	–0.150942000
C	1.117446000	4.089818000	–0.195449000
H	0.163638000	3.790234000	0.233287000
H	0.939817000	4.397212000	–1.232228000
H	1.490624000	4.962249000	0.342939000

*Coordinates of the geometry of isomer **ttt** of* **BT** *optimized with the B3LYP functional*

S	–5.863726000	–1.550706000	0.446418000
F	–0.241486000	1.611109000	1.141495000
F	–0.276883000	1.742487000	–1.149538000
N	–4.608296000	0.617165000	–0.294193000
N	0.470557000	–0.335494000	–0.122761000
N	1.877426000	1.724560000	–0.041664000
B	0.424447000	1.205491000	–0.041508000
C	–6.815370000	–0.121453000	0.118627000
C	–8.198076000	0.055899000	0.189039000
H	–8.852787000	–0.755575000	0.482026000
C	–8.714268000	1.307691000	–0.128544000
H	–9.784819000	1.469094000	–0.081314000
C	–7.868045000	2.364184000	–0.509206000
H	–8.297944000	3.329242000	–0.750886000
C	–6.493863000	2.188827000	–0.579650000
H	–5.835860000	2.998404000	–0.872324000
C	–5.949469000	0.933451000	–0.264115000
C	–4.394503000	–0.622515000	0.045859000
C	–3.107161000	–1.283627000	0.121792000
H	–3.127519000	–2.323776000	0.414233000
C	–1.944891000	–0.634638000	–0.129610000
H	–2.015799000	0.419188000	–0.368261000

C	–0.610158000	–1.177475000	–0.110875000
C	–0.143629000	–2.521517000	–0.125464000
C	–0.981412000	–3.771087000	–0.163557000
H	–0.448433000	–4.538252000	–0.731253000
H	–1.899382000	–3.580638000	–0.725089000
C	–1.327270000	–4.337682000	1.226605000
H	–0.420388000	–4.613903000	1.770677000
H	–1.951540000	–5.230480000	1.133609000
H	–1.866448000	–3.609481000	1.838153000
C	1.253155000	–2.476715000	–0.133998000
C	2.142610000	–3.685205000	–0.150536000
H	1.554415000	–4.592475000	–0.015506000
H	2.888530000	–3.651481000	0.644846000
H	2.685955000	–3.777478000	–1.094221000
C	1.629461000	–1.096823000	–0.131033000
C	2.902256000	–0.474316000	–0.129376000
C	4.135158000	–1.318172000	–0.165231000
C	4.645055000	–1.772236000	–1.385795000
H	4.140894000	–1.510962000	–2.309436000
C	5.799697000	–2.552365000	–1.418451000
H	6.188837000	–2.895872000	–2.370193000
C	6.450765000	–2.890745000	–0.232160000
H	7.347172000	–3.499742000	–0.258207000
C	5.944018000	–2.442483000	0.987555000
H	6.444559000	–2.701641000	1.913563000
C	4.792734000	–1.657291000	1.021467000
H	4.401834000	–1.308552000	1.970738000
C	3.021608000	0.914405000	–0.096757000
C	4.167130000	1.786550000	–0.118534000
C	5.617103000	1.414906000	–0.178452000
H	6.230373000	2.305800000	–0.316619000
H	5.828837000	0.726267000	–0.998108000
H	5.945079000	0.924732000	0.741831000
C	3.681025000	3.090230000	–0.076795000
C	4.474511000	4.368321000	–0.064539000
H	3.883995000	5.165622000	–0.524705000
H	5.360743000	4.252978000	–0.695025000
C	4.911065000	4.809242000	1.344823000
H	4.045867000	4.967998000	1.994320000
H	5.475848000	5.744448000	1.299045000
H	5.545404000	4.052398000	1.813842000
C	2.263598000	3.014166000	–0.026615000
C	1.305802000	4.157510000	0.003513000
H	0.367647000	3.881783000	0.481410000
H	1.079042000	4.490802000	–1.015430000
H	1.738978000	5.005182000	0.535934000

*Coordinates of the geometry of isomer **ttc** of* **BT** *optimized with the B3LYP functional*

S	–4.650354000	1.121186000	–0.493673000
F	–0.209604000	1.644887000	1.110773000
F	–0.224448000	1.759312000	–1.180344000
N	–5.521615000	–1.193752000	0.357320000
N	0.473465000	–0.324673000	–0.133188000
N	1.921855000	1.705547000	–0.055156000
B	0.459213000	1.217110000	–0.062866000

C	–6.372031000	0.925607000	–0.244544000
C	–7.399246000	1.849562000	–0.437642000
H	–7.192838000	2.853511000	–0.787476000
C	–8.702572000	1.444073000	–0.166852000
H	–9.517058000	2.144594000	–0.309367000
C	–8.976949000	0.142619000	0.287427000
H	–10.001765000	–0.145388000	0.490455000
C	–7.954776000	–0.776091000	0.479076000
H	–8.157398000	–1.781250000	0.829400000
C	–6.632625000	–0.388535000	0.212104000
C	–4.420905000	–0.568399000	0.038968000
C	–3.120246000	–1.194600000	0.113309000
H	–3.161707000	–2.224489000	0.440149000
C	–1.948808000	–0.573628000	–0.158893000
H	–1.979052000	0.475716000	–0.429733000
C	–0.624274000	–1.143261000	–0.123117000
C	–0.187958000	–2.496830000	–0.122380000
C	–1.052471000	–3.728091000	–0.159797000
H	–0.537188000	–4.505852000	–0.729516000
H	–1.967506000	–3.517047000	–0.718641000
C	–1.408095000	–4.288509000	1.230337000
H	–0.506646000	–4.584141000	1.773245000
H	–2.051145000	–5.167826000	1.137180000
H	–1.931512000	–3.549699000	1.842889000
C	1.209907000	–2.482054000	–0.119630000
C	2.072915000	–3.709611000	–0.119300000
H	1.462439000	–4.604009000	0.001881000
H	2.802114000	–3.692535000	0.692178000
H	2.634311000	–3.812785000	–1.051031000
C	1.615943000	–1.110887000	–0.124728000
C	2.901396000	–0.515207000	–0.115865000
C	4.116294000	–1.385459000	–0.132101000
C	4.630513000	–1.858372000	–1.343692000
H	4.143378000	–1.591775000	–2.274917000
C	5.767605000	–2.664360000	–1.357681000
H	6.160195000	–3.022583000	–2.302554000
C	6.396860000	–3.009494000	–0.161586000
H	7.279805000	–3.638282000	–0.173094000
C	5.885920000	–2.542070000	1.049139000
H	6.369608000	–2.806201000	1.982664000
C	4.752085000	–1.731298000	1.064426000
H	4.357802000	–1.367928000	2.006785000
C	3.049233000	0.871014000	–0.093199000
C	4.212766000	1.718785000	–0.110575000
C	5.655095000	1.316480000	–0.153873000
H	6.288039000	2.192723000	–0.297007000
H	5.859156000	0.614078000	–0.963641000
H	5.965037000	0.830438000	0.774880000
C	3.753977000	3.032813000	–0.083160000
C	4.575089000	4.293353000	–0.072461000
H	4.005066000	5.101100000	–0.540119000
H	5.462366000	4.155257000	–0.696918000
C	5.012612000	4.731620000	1.337432000
H	4.147073000	4.911472000	1.980929000
H	5.597213000	5.654512000	1.290710000

H	5.628142000	3.963901000	1.813780000
C	2.335062000	2.987055000	–0.045951000
C	1.400336000	4.149635000	–0.032880000
H	0.458348000	3.900054000	0.452074000
H	1.176604000	4.469668000	–1.056697000
H	1.851339000	4.997428000	0.484055000

*Coordinates of the geometry of isomer **ctt** of* **BT** *optimized with the M06HF functional*

S	–4.958444000	1.784274000	–0.032015000
F	–0.279792000	1.553397000	1.118480000
F	–0.313760000	1.622681000	–1.176565000
N	–4.925811000	–0.797979000	–0.060440000
N	0.424157000	–0.427627000	–0.094901000
N	1.820891000	1.641382000	–0.068348000
B	0.368792000	1.105835000	–0.054227000
C	–6.485849000	0.959524000	–0.043671000
C	–7.777029000	1.490842000	–0.041123000
H	–7.939411000	2.558532000	–0.030350000
C	–8.839039000	0.604321000	–0.053162000
H	–9.849063000	0.987135000	–0.051754000
C	–8.624507000	–0.785306000	–0.067242000
H	–9.475144000	–1.451391000	–0.076248000
C	–7.345856000	–1.308278000	–0.069982000
H	–7.165688000	–2.373423000	–0.081152000
C	–6.259994000	–0.424189000	–0.058335000
C	–4.148073000	0.225677000	–0.048403000
C	–2.676471000	0.186275000	–0.050533000
H	–2.165648000	1.135290000	–0.028245000
C	–2.047569000	–0.993243000	–0.082015000
H	–2.672914000	–1.877725000	–0.096044000
C	–0.619669000	–1.297136000	–0.089418000
C	–0.125500000	–2.611670000	–0.079687000
C	–0.942198000	–3.879572000	–0.040525000
H	–0.372767000	–4.678202000	–0.513602000
H	–1.852672000	–3.757320000	–0.624837000
C	–1.299909000	–4.280093000	1.405956000
H	–0.389689000	–4.426053000	1.987672000
H	–1.877077000	–5.204256000	1.413569000
H	–1.886789000	–3.491491000	1.877213000
C	1.274806000	–2.534899000	–0.057871000
C	2.187491000	–3.738745000	–0.012072000
H	1.654192000	–4.568903000	0.447582000
H	3.087220000	–3.537850000	0.563501000
H	2.483176000	–4.030961000	–1.020567000
C	1.592732000	–1.163682000	–0.083924000
C	2.866300000	–0.518603000	–0.105970000
C	4.103182000	–1.349094000	–0.128930000
C	4.518675000	–1.943544000	–1.317004000
H	3.942353000	–1.799830000	–2.221059000
C	5.677857000	–2.711504000	–1.330527000
H	6.008793000	–3.168295000	–2.252033000
C	6.407054000	–2.894769000	–0.158486000
H	7.305002000	–3.496434000	–0.170549000
C	5.982965000	–2.304329000	1.028441000
H	6.545318000	–2.448277000	1.939544000

C	4.831128000	–1.525186000	1.044231000
H	4.493217000	–1.058437000	1.959817000
C	2.971232000	0.842565000	–0.109045000
C	4.112592000	1.733398000	–0.182245000
C	5.569618000	1.360844000	–0.249908000
H	6.150218000	2.237714000	–0.528822000
H	5.735831000	0.568048000	–0.977563000
H	5.910844000	1.006988000	0.722814000
C	3.612144000	3.010676000	–0.180553000
C	4.372137000	4.310667000	–0.206622000
H	3.720742000	5.097607000	–0.583664000
H	5.209007000	4.226427000	–0.898152000
C	4.889020000	4.685209000	1.197669000
H	4.054639000	4.777487000	1.892858000
H	5.426454000	5.631908000	1.162877000
H	5.560854000	3.909673000	1.564934000
C	2.178491000	2.908540000	–0.103480000
C	1.210723000	4.052204000	–0.093357000
H	0.223667000	3.723108000	0.214342000
H	1.158206000	4.473625000	–1.098799000
H	1.576652000	4.821216000	0.585433000

*Coordinates of the geometry of isomer **ctc** of* **BT** *optimized with the M06HF functional*

S	–5.162196000	–1.315147000	–0.161378000
F	–0.302446000	1.499879000	1.163646000
F	–0.401894000	1.570191000	–1.130893000
N	–4.774378000	1.232002000	0.088699000
N	0.438631000	–0.451652000	–0.074511000
N	1.758748000	1.666961000	–0.076036000
B	0.328694000	1.078930000	–0.029467000
C	–6.561886000	–0.279943000	–0.108600000
C	–7.911653000	–0.623027000	–0.188950000
H	–8.219638000	–1.652207000	–0.299027000
C	–8.841246000	0.400931000	–0.126045000
H	–9.893888000	0.166099000	–0.188019000
C	–8.438633000	1.739548000	0.015829000
H	–9.187975000	2.516171000	0.064212000
C	–7.100019000	2.074508000	0.094640000
H	–6.773551000	3.098532000	0.203189000
C	–6.149205000	1.050707000	0.030096000
C	–4.143031000	0.115222000	–0.000415000
C	–2.677494000	0.044572000	0.027881000
H	–2.199492000	1.003023000	0.155518000
C	–2.011363000	–1.107315000	–0.094174000
H	–2.580771000	–2.023072000	–0.204529000
C	–0.571925000	–1.358548000	–0.085892000
C	–0.031292000	–2.653979000	–0.079379000
C	–0.803655000	–3.949841000	–0.057487000
H	–0.180388000	–4.734313000	–0.483003000
H	–1.684641000	–3.874599000	–0.694020000
C	–1.224489000	–4.338309000	1.375026000
H	–0.342843000	–4.423583000	2.010614000
H	–1.753518000	–5.290591000	1.371466000
H	–1.877897000	–3.572881000	1.794387000
C	1.365374000	–2.526317000	–0.038649000

C	2.320532000	–3.696340000	0.017146000
H	1.818352000	–4.539815000	0.487748000
H	3.213870000	–3.458371000	0.588565000
H	2.623746000	–3.989069000	–0.988983000
C	1.633151000	–1.144834000	–0.056157000
C	2.882462000	–0.453202000	–0.085133000
C	4.150026000	–1.236357000	–0.108265000
C	4.582888000	–1.818081000	–1.296583000
H	3.996411000	–1.701172000	–2.198037000
C	5.771774000	–2.538865000	–1.313741000
H	6.116025000	–2.985259000	–2.235560000
C	6.513788000	–2.688652000	–0.145029000
H	7.434796000	–3.253733000	–0.160124000
C	6.072456000	–2.111316000	1.042074000
H	6.645221000	–2.228377000	1.950569000
C	4.889937000	–1.379607000	1.061668000
H	4.538712000	–0.923072000	1.977447000
C	2.937754000	0.910651000	–0.106352000
C	4.044895000	1.842661000	–0.198017000
C	5.514733000	1.523255000	–0.260279000
H	6.063299000	2.416589000	–0.550487000
H	5.710276000	0.727132000	–0.976840000
H	5.867355000	1.194814000	0.717297000
C	3.497037000	3.099975000	–0.217053000
C	4.206647000	4.427353000	–0.266728000
H	3.526301000	5.180898000	–0.661158000
H	5.048787000	4.362446000	–0.953902000
C	4.703803000	4.849943000	1.131256000
H	3.864205000	4.924374000	1.822329000
H	5.204468000	5.815823000	1.077721000
H	5.404095000	4.108579000	1.516158000
C	2.068107000	2.945732000	–0.133262000
C	1.057616000	4.051564000	–0.135872000
H	0.085416000	3.689839000	0.182863000
H	0.982880000	4.453879000	–1.147737000
H	1.397562000	4.845261000	0.527567000

*Coordinates of the geometry of isomer **ttt** of* **BT** *optimized with the M06HF functional*

S	–5.812199000	–1.514850000	0.547738000
F	–0.272398000	1.595919000	1.112883000
F	–0.267761000	1.758494000	–1.172300000
N	–4.589654000	0.592866000	–0.312838000
N	0.464251000	–0.327223000	–0.159949000
N	1.863075000	1.721718000	–0.036337000
B	0.404965000	1.203809000	–0.061288000
C	–6.778408000	–0.120631000	0.163183000
C	–8.161547000	0.048035000	0.250642000
H	–8.798636000	–0.753239000	0.594754000
C	–8.685730000	1.274629000	–0.115781000
H	–9.752187000	1.436005000	–0.056875000
C	–7.852775000	2.315579000	–0.563130000
H	–8.292524000	3.261892000	–0.841807000
C	–6.485024000	2.144973000	–0.649884000
H	–5.832780000	2.935518000	–0.991425000
C	–5.938642000	0.909791000	–0.281724000

C	–4.379960000	–0.610754000	0.085217000
C	–3.063658000	–1.263362000	0.172985000
H	–3.050787000	–2.273515000	0.553332000
C	–1.956106000	–0.607650000	–0.184140000
H	–2.049868000	0.418572000	–0.517612000
C	–0.602489000	–1.160971000	–0.160280000
C	–0.148744000	–2.492449000	–0.173277000
C	–0.988685000	–3.743720000	–0.209938000
H	–0.464687000	–4.501002000	–0.791392000
H	–1.922291000	–3.538334000	–0.731448000
C	–1.269804000	–4.294768000	1.204474000
H	–0.333273000	–4.575874000	1.685416000
H	–1.914474000	–5.171797000	1.150993000
H	–1.749547000	–3.539480000	1.826957000
C	1.254054000	–2.448473000	–0.161005000
C	2.148266000	–3.666498000	–0.170326000
H	1.569232000	–4.538035000	0.128206000
H	2.983969000	–3.548676000	0.516549000
H	2.549424000	–3.839422000	–1.169194000
C	1.613161000	–1.084303000	–0.155473000
C	2.890135000	–0.454352000	–0.135836000
C	4.116068000	–1.300533000	–0.159873000
C	4.544412000	–1.869341000	–1.355910000
H	3.986553000	–1.691935000	–2.265674000
C	5.692639000	–2.653436000	–1.369997000
H	6.034034000	–3.089909000	–2.297664000
C	6.398355000	–2.877852000	–0.190526000
H	7.288390000	–3.491250000	–0.203058000
C	5.961182000	–2.313512000	1.004335000
H	6.505795000	–2.489752000	1.920587000
C	4.820050000	–1.518710000	1.021060000
H	4.471998000	–1.071340000	1.942583000
C	3.005032000	0.908289000	–0.090769000
C	4.156004000	1.785425000	–0.123345000
C	5.609262000	1.396809000	–0.188081000
H	6.201885000	2.271140000	–0.449464000
H	5.771542000	0.613782000	–0.927074000
H	5.940226000	1.023831000	0.781148000
C	3.672082000	3.070232000	–0.087465000
C	4.450181000	4.359753000	–0.068754000
H	3.813214000	5.166329000	–0.428673000
H	5.292050000	4.284035000	–0.755288000
C	4.959526000	4.687237000	1.349794000
H	4.119840000	4.772720000	2.039504000
H	5.511488000	5.626214000	1.346681000
H	5.615922000	3.891442000	1.701176000
C	2.239037000	2.985087000	–0.027112000
C	1.281750000	4.137335000	0.011396000
H	0.293878000	3.809298000	0.318748000
H	1.224926000	4.579228000	–0.984989000
H	1.657014000	4.889708000	0.703519000

*Coordinates of the geometry of isomer **ttc** of* **BT** *optimized with the M06HF functional*

S	–4.652151000	0.991425000	–0.694836000
F	–0.284499000	1.616741000	1.034158000

F	–0.212875000	1.751679000	–1.250109000
N	–5.447673000	–1.137151000	0.544898000
N	0.469098000	–0.328391000	–0.193204000
N	1.886459000	1.704904000	–0.053976000
B	0.424486000	1.203653000	–0.114041000
C	–6.343881000	0.859579000	–0.310009000
C	–7.378211000	1.756232000	–0.579902000
H	–7.188497000	2.687287000	–1.093121000
C	–8.653342000	1.412594000	–0.164534000
H	–9.473620000	2.087990000	–0.359164000
C	–8.897640000	0.201326000	0.504782000
H	–9.903705000	–0.037947000	0.816948000
C	–7.870417000	–0.685082000	0.768241000
H	–8.042321000	–1.620949000	1.279773000
C	–6.576525000	–0.351187000	0.354123000
C	–4.395183000	–0.576469000	0.064971000
C	–3.066788000	–1.194895000	0.151071000
H	–3.069106000	–2.178195000	0.597341000
C	–1.953164000	–0.578120000	–0.251495000
H	–2.006614000	0.430947000	–0.645050000
C	–0.607067000	–1.149197000	–0.196496000
C	–0.171781000	–2.485582000	–0.181507000
C	–1.029979000	–3.724556000	–0.208959000
H	–0.522530000	–4.490369000	–0.794227000
H	–1.965935000	–3.504580000	–0.720329000
C	–1.307374000	–4.269257000	1.208538000
H	–0.371140000	–4.557238000	1.686015000
H	–1.959986000	–5.140631000	1.160486000
H	–1.778072000	–3.508133000	1.830702000
C	1.231968000	–2.458637000	–0.152491000
C	2.110448000	–3.687907000	–0.136324000
H	1.514348000	–4.550621000	0.154099000
H	2.933252000	–3.576608000	0.567121000
H	2.529915000	–3.870893000	–1.125799000
C	1.608319000	–1.099397000	–0.161192000
C	2.892010000	–0.483070000	–0.123202000
C	4.107082000	–1.345000000	–0.119904000
C	4.545994000	–1.928911000	–1.304888000
H	4.005593000	–1.749565000	–2.224708000
C	5.680606000	–2.732425000	–1.294564000
H	6.029589000	–3.181092000	–2.213474000
C	6.363121000	–2.960181000	–0.102136000
H	7.242699000	–3.588570000	–0.096179000
C	5.916078000	–2.379687000	1.081333000
H	6.443194000	–2.557760000	2.007398000
C	4.788506000	–1.565582000	1.073751000
H	4.432763000	–1.106626000	1.986496000
C	3.020453000	0.878512000	–0.083110000
C	4.181252000	1.743271000	–0.093616000
C	5.631051000	1.338400000	–0.126842000
H	6.238273000	2.204609000	–0.381747000
H	5.799372000	0.549157000	–0.857737000
H	5.938579000	0.968159000	0.851033000
C	3.710936000	3.033384000	–0.069449000
C	4.501679000	4.314773000	–0.032865000

H	3.882030000	5.127600000	–0.408640000
H	5.359566000	4.230141000	–0.698284000
C	4.979222000	4.637848000	1.397821000
H	4.123866000	4.727538000	2.067593000
H	5.536692000	5.573517000	1.408781000
H	5.622358000	3.837769000	1.763606000
C	2.276354000	2.964084000	–0.039526000
C	1.331061000	4.126697000	–0.025266000
H	0.333446000	3.810438000	0.262385000
H	1.300649000	4.565283000	–1.024230000
H	1.699775000	4.877646000	0.671898000

*Coordinates of the geometry of isomer **ctt** of* **NBT** *optimized with the B3LYP functional*

S	–4.255738000	1.513281000	0.052279000
F	0.456274000	1.512764000	1.087770000
F	0.403138000	1.532337000	–1.211314000
N	–4.140079000	–1.096916000	–0.090653000
N	1.232719000	–0.463920000	–0.093699000
N	2.548985000	1.669037000	–0.112282000
B	1.124053000	1.075700000	–0.083618000
C	–5.755656000	0.621120000	0.000658000
C	–7.057464000	1.098706000	0.023511000
H	–7.288941000	2.152539000	0.080367000
C	–8.077694000	0.151618000	–0.031084000
C	–7.831162000	–1.230052000	–0.105498000
H	–8.664905000	–1.916046000	–0.144819000
C	–6.530013000	–1.691683000	–0.127332000
H	–6.316995000	–2.751551000	–0.184194000
C	–5.467969000	–0.770080000	–0.074877000
C	–3.376747000	–0.033319000	–0.030987000
C	–1.934594000	–0.009566000	–0.026966000
H	–1.469065000	0.961519000	0.031410000
C	–1.206665000	–1.154176000	–0.088063000
H	–1.782718000	–2.071337000	–0.132226000
C	0.210959000	–1.382850000	–0.095058000
C	0.770507000	–2.690547000	–0.099413000
C	–0.001955000	–3.982429000	–0.082928000
H	0.570030000	–4.747390000	–0.614013000
H	–0.930926000	–3.871095000	–0.647965000
C	–0.326670000	–4.488208000	1.334841000
H	0.586820000	–4.656082000	1.911509000
H	–0.877259000	–5.431705000	1.289215000
H	–0.937799000	–3.764873000	1.881065000
C	2.160155000	–2.557798000	–0.085872000
C	3.124257000	–3.707915000	–0.067291000
H	2.585380000	–4.650483000	0.025669000
H	3.822786000	–3.641258000	0.768150000
H	3.721979000	–3.754016000	–0.980378000
C	2.437629000	–1.157451000	–0.091778000
C	3.681537000	–0.468297000	–0.103013000
C	4.957220000	–1.247324000	–0.105699000
C	5.526126000	–1.666468000	–1.312447000
H	5.034363000	–1.430298000	–2.249454000
C	6.722364000	–2.381984000	–1.313766000
H	7.156535000	–2.700260000	–2.254686000

C	7.357636000	–2.687096000	–0.110075000
H	8.287018000	–3.245042000	–0.111740000
C	6.792652000	–2.272017000	1.095669000
H	7.281232000	–2.505275000	2.034823000
C	5.598237000	–1.553363000	1.098764000
H	5.161886000	–1.230723000	2.037398000
C	3.733134000	0.919779000	–0.116351000
C	4.835576000	1.851538000	–0.151046000
C	6.302613000	1.552548000	–0.164774000
H	6.875402000	2.474167000	–0.268837000
H	6.574769000	0.887593000	–0.986487000
H	6.621219000	1.063234000	0.758877000
C	4.281905000	3.124901000	–0.171274000
C	5.002442000	4.445066000	–0.195923000
H	4.379276000	5.187516000	–0.702412000
H	5.908840000	4.354238000	–0.800980000
C	5.378679000	4.967390000	1.203105000
H	4.491160000	5.104499000	1.826810000
H	5.891876000	5.929985000	1.129239000
H	6.042340000	4.267424000	1.717381000
C	2.866148000	2.974844000	–0.144100000
C	1.856695000	4.071349000	–0.184186000
H	0.895949000	3.752796000	0.213424000
H	1.703429000	4.402264000	–1.217653000
H	2.209228000	4.934176000	0.383155000
N	–9.460728000	0.620132000	–0.009552000
O	–10.362147000	–0.216607000	–0.061171000
O	–9.668060000	1.831964000	0.059135000

*Coordinates of the geometry of isomer **ctc** of* **NBT** *optimized with the B3LYP functional*

S	–4.403248000	–1.332816000	–0.134677000
F	0.479728000	1.553257000	1.083291000
F	0.425365000	1.570238000	–1.216321000
N	–4.022793000	1.253064000	0.049463000
N	1.230254000	–0.434486000	–0.096844000
N	2.572847000	1.682237000	–0.117943000
B	1.140523000	1.106916000	–0.088340000
C	–5.803289000	–0.289244000	–0.060818000
C	–7.146038000	–0.634321000	–0.083634000
H	–7.483156000	–1.658194000	–0.155395000
C	–8.065578000	0.410044000	–0.008527000
C	–7.682716000	1.758006000	0.085494000
H	–8.443054000	2.523534000	0.140146000
C	–6.340725000	2.085941000	0.106868000
H	–6.021333000	3.117781000	0.179152000
C	–5.379239000	1.062763000	0.034621000
C	–3.367716000	0.119535000	–0.029401000
C	–1.929104000	0.058721000	–0.027871000
H	–1.453109000	1.024248000	0.045572000
C	–1.217575000	–1.093847000	–0.100768000
H	–1.786872000	–2.016075000	–0.157881000
C	0.198171000	–1.340983000	–0.103291000
C	0.741088000	–2.655268000	–0.105229000
C	–0.047248000	–3.937748000	–0.093672000
H	0.524584000	–4.712622000	–0.610065000

H	–0.964362000	–3.820038000	–0.676949000
C	–0.403161000	–4.431198000	1.321024000
H	0.498082000	–4.606348000	1.914470000
H	–0.963931000	–5.368415000	1.270919000
H	–1.015031000	–3.697779000	1.852860000
C	2.132297000	–2.539397000	–0.083426000
C	3.081707000	–3.701523000	–0.058367000
H	2.531580000	–4.635762000	0.051096000
H	3.788383000	–3.633528000	0.769826000
H	3.670378000	–3.766918000	–0.976313000
C	2.426829000	–1.142784000	–0.088999000
C	3.679120000	–0.468623000	–0.098069000
C	4.945184000	–1.263206000	–0.093187000
C	5.511270000	–1.697616000	–1.295822000
H	5.024475000	–1.461661000	–2.235463000
C	6.698682000	–2.427660000	–1.289751000
H	7.130832000	–2.757610000	–2.227576000
C	7.327721000	–2.732327000	–0.082691000
H	8.250161000	–3.301664000	–0.078578000
C	6.765498000	–2.301991000	1.119011000
H	7.249279000	–2.534781000	2.060761000
C	5.580038000	–1.568728000	1.114711000
H	5.145779000	–1.234280000	2.050174000
C	3.747731000	0.918470000	–0.116579000
C	4.861640000	1.836648000	–0.152967000
C	6.324881000	1.519659000	–0.164173000
H	6.909035000	2.433878000	–0.270347000
H	6.589572000	0.849165000	–0.983879000
H	6.636575000	1.029000000	0.761088000
C	4.323620000	3.116466000	–0.178976000
C	5.060458000	4.427514000	–0.207762000
H	4.446708000	5.175945000	–0.716945000
H	5.965851000	4.323294000	–0.812159000
C	5.442573000	4.949794000	1.189715000
H	4.556502000	5.099954000	1.812462000
H	5.967674000	5.905705000	1.112859000
H	6.097291000	4.243379000	1.706636000
C	2.905942000	2.983827000	–0.153629000
C	1.910298000	4.092671000	–0.198069000
H	0.943956000	3.786344000	0.195555000
H	1.765565000	4.425394000	–1.232180000
H	2.271322000	4.951097000	0.370681000
N	–9.490001000	0.082643000	–0.028633000
O	–10.302014000	1.004561000	0.042413000
O	–9.817428000	–1.100784000	–0.115366000

*Coordinates of the geometry of isomer **ttt** of* **NBT** *optimized with the B3LYP functional*

S	–4.983254000	–1.989352000	0.368851000
F	0.437868000	1.510515000	1.125974000
F	0.391120000	1.632121000	–1.164945000
N	–3.834946000	0.277124000	–0.257376000
N	1.267276000	–0.391691000	–0.133410000
N	2.543644000	1.752039000	–0.060052000
B	1.124700000	1.144310000	–0.056760000
C	–5.998153000	–0.593154000	0.105450000

C	–7.379321000	–0.491777000	0.178351000
H	–8.011753000	–1.331894000	0.426015000
C	–7.934068000	0.758693000	–0.084399000
C	–7.157366000	1.883671000	–0.409933000
H	–7.646094000	2.827614000	–0.603101000
C	–5.783019000	1.768360000	–0.478306000
H	–5.164815000	2.621587000	–0.726710000
C	–5.180165000	0.523582000	–0.220905000
C	–3.562780000	–0.972103000	0.024763000
C	–2.248662000	–1.567281000	0.079507000
H	–2.213793000	–2.618581000	0.324798000
C	–1.122562000	–0.840670000	–0.135832000
H	–1.256789000	0.215968000	–0.330525000
C	0.239215000	–1.300838000	–0.127764000
C	0.789313000	–2.612610000	–0.149736000
C	0.032796000	–3.912509000	–0.194244000
H	0.620151000	–4.645309000	–0.753183000
H	–0.888227000	–3.782858000	–0.767819000
C	–0.291550000	–4.495852000	1.194198000
H	0.625364000	–4.709352000	1.749481000
H	–0.853926000	–5.428373000	1.097255000
H	–0.885095000	–3.803159000	1.796516000
C	2.180864000	–2.479549000	–0.153215000
C	3.146411000	–3.628065000	–0.176187000
H	2.616714000	–4.573733000	–0.064316000
H	3.878071000	–3.560226000	0.630206000
H	3.706967000	–3.668423000	–1.113261000
C	2.467629000	–1.078985000	–0.140379000
C	3.703561000	–0.377806000	–0.127382000
C	4.985622000	–1.145394000	–0.147095000
C	5.545207000	–1.556672000	–1.360931000
H	5.043859000	–1.318684000	–2.292365000
C	6.745147000	–2.265790000	–1.376313000
H	7.172689000	–2.577020000	–2.322610000
C	7.392174000	–2.574534000	–0.179829000
H	8.323949000	–3.128329000	–0.192616000
C	6.835716000	–2.168768000	1.033025000
H	7.333079000	–2.405417000	1.966705000
C	5.638650000	–1.454767000	1.050201000
H	5.209044000	–1.138885000	1.994199000
C	3.736415000	1.012301000	–0.095969000
C	4.828535000	1.954939000	–0.107554000
C	6.298387000	1.670758000	–0.141848000
H	6.859921000	2.597814000	–0.258803000
H	6.565866000	1.004049000	–0.963333000
H	6.635656000	1.190723000	0.780303000
C	4.263498000	3.224197000	–0.082378000
C	4.973104000	4.550457000	–0.067845000
H	4.340943000	5.303953000	–0.545995000
H	5.876396000	4.487435000	–0.681110000
C	5.354162000	5.029733000	1.345083000
H	4.469234000	5.140136000	1.977741000
H	5.860111000	5.997948000	1.299712000
H	6.025816000	4.318332000	1.832660000
C	2.850376000	3.060903000	–0.050260000

C	1.827425000	4.145775000	–0.043887000
H	0.887708000	3.811530000	0.390848000
H	1.625636000	4.479541000	–1.068017000
H	2.191023000	5.009644000	0.514226000
N	–9.386365000	0.901332000	–0.016946000
O	–9.876416000	2.005526000	–0.252406000
O	–10.059416000	–0.088120000	0.272429000

*Coordinates of the geometry of isomer **ttc** of* **NBT** *optimized with the B3LYP functional*

S	–3.957038000	0.593040000	–0.341890000
F	0.411522000	1.478413000	1.139997000
F	0.356984000	1.600790000	–1.149720000
N	–4.635773000	–1.846344000	0.331336000
N	1.256720000	–0.413994000	–0.122834000
N	2.512723000	1.741290000	–0.051570000
B	1.100519000	1.120277000	–0.044064000
C	–5.653198000	0.231860000	–0.122349000
C	–6.745498000	1.075259000	–0.258749000
H	–6.646860000	2.115927000	–0.531370000
C	–8.001902000	0.519549000	–0.027285000
C	–8.187179000	–0.826230000	0.328985000
H	–9.187533000	–1.198461000	0.495779000
C	–7.088945000	–1.654031000	0.461174000
H	–7.206451000	–2.694669000	0.735257000
C	–5.802568000	–1.134056000	0.235700000
C	–3.588095000	–1.104079000	0.067447000
C	–2.244556000	–1.623349000	0.107515000
H	–2.200042000	–2.672365000	0.363634000
C	–1.129756000	–0.885749000	–0.119521000
H	–1.255081000	0.171572000	–0.323937000
C	0.237681000	–1.332539000	–0.114532000
C	0.798655000	–2.639180000	–0.138939000
C	0.054452000	–3.946206000	–0.183021000
H	0.645140000	–4.670871000	–0.749040000
H	–0.872064000	–3.823501000	–0.749138000
C	–0.254392000	–4.538102000	1.205267000
H	0.668257000	–4.742724000	1.754391000
H	–0.806400000	–5.476755000	1.108194000
H	–0.852780000	–3.854723000	1.813405000
C	2.189269000	–2.493199000	–0.147001000
C	3.165137000	–3.632822000	–0.174542000
H	2.644337000	–4.583742000	–0.065558000
H	3.896700000	–3.560854000	0.631638000
H	3.725397000	–3.664714000	–1.112067000
C	2.463429000	–1.090435000	–0.134290000
C	3.692616000	–0.377603000	–0.125497000
C	4.981599000	–1.133287000	–0.151047000
C	5.539732000	–1.538608000	–1.367568000
H	5.032376000	–1.304430000	–2.296713000
C	6.745755000	–2.237161000	–1.388454000
H	7.172110000	–2.543892000	–2.336750000
C	7.400333000	–2.541207000	–0.194875000
H	8.336863000	–3.086796000	–0.211974000
C	6.845364000	–2.141334000	1.020602000
H	7.348625000	–2.374390000	1.952017000

C	5.642194000	–1.437805000	1.043317000
H	5.213728000	–1.126490000	1.989342000
C	3.712338000	1.012758000	–0.092902000
C	4.795273000	1.965715000	–0.108279000
C	6.267589000	1.695428000	–0.148364000
H	6.819773000	2.627308000	–0.271238000
H	6.537697000	1.028114000	–0.968426000
H	6.613498000	1.222218000	0.774152000
C	4.218420000	3.229691000	–0.079956000
C	4.915690000	4.562506000	–0.067465000
H	4.274499000	5.310442000	–0.542263000
H	5.816764000	4.508417000	–0.684818000
C	5.298586000	5.044229000	1.344110000
H	4.415496000	5.146185000	1.980739000
H	5.795529000	6.017017000	1.297152000
H	5.978823000	4.338653000	1.828224000
C	2.807192000	3.053133000	–0.042129000
C	1.773562000	4.127781000	–0.031137000
H	0.842271000	3.786689000	0.416434000
H	1.556550000	4.452611000	–1.055013000
H	2.134445000	4.998811000	0.517347000
N	–9.176697000	1.379456000	–0.164366000
O	–10.286262000	0.887849000	0.038242000
O	–9.006195000	2.557666000	–0.476565000

*Coordinates of the geometry of isomer **ctt** of* **NBT** *optimized with the M06HF functional*

S	–4.235882000	1.506658000	–0.007981000
F	0.440238000	1.474693000	1.129737000
F	0.386127000	1.544417000	–1.164900000
N	–4.103431000	–1.074944000	–0.049430000
N	1.223144000	–0.469925000	–0.090629000
N	2.526085000	1.658521000	–0.071406000
B	1.099907000	1.058655000	–0.048521000
C	–5.724529000	0.620441000	–0.025488000
C	–7.028852000	1.101627000	–0.021721000
H	–7.263215000	2.155441000	–0.004965000
C	–8.022512000	0.146002000	–0.040462000
C	–7.789452000	–1.233599000	–0.062750000
H	–8.625119000	–1.915490000	–0.076568000
C	–6.489905000	–1.689765000	–0.065788000
H	–6.266565000	–2.745931000	–0.082222000
C	–5.444139000	–0.757250000	–0.047792000
C	–3.367512000	–0.016205000	–0.030227000
C	–1.899206000	0.009365000	–0.029462000
H	–1.431519000	0.979915000	0.010599000
C	–1.220838000	–1.142953000	–0.078935000
H	–1.807656000	–2.053050000	–0.108246000
C	0.216891000	–1.384775000	–0.087461000
C	0.767561000	–2.675343000	–0.079968000
C	0.008492000	–3.978423000	–0.042075000
H	0.616170000	–4.751025000	–0.510372000
H	–0.904021000	–3.899652000	–0.630997000
C	–0.336753000	–4.391733000	1.403870000
H	0.576075000	–4.487054000	1.992033000
H	–0.864971000	–5.344422000	1.411413000

H	–0.967673000	–3.633493000	1.867907000
C	2.164518000	–2.536886000	–0.056719000
C	3.128990000	–3.699868000	–0.013231000
H	2.632636000	–4.553330000	0.444931000
H	4.019339000	–3.462219000	0.563278000
H	3.437005000	–3.977466000	–1.022176000
C	2.420258000	–1.154135000	–0.079748000
C	3.667511000	–0.451801000	–0.101928000
C	4.939665000	–1.227131000	–0.128229000
C	5.377152000	–1.800306000	–1.318992000
H	4.791651000	–1.681404000	–2.220794000
C	6.569390000	–2.515475000	–1.337907000
H	6.917406000	–2.955200000	–2.261561000
C	7.310048000	–2.668205000	–0.168704000
H	8.233544000	–3.229097000	–0.185251000
C	6.864086000	–2.099391000	1.020791000
H	7.435747000	–2.218889000	1.929651000
C	5.678094000	–1.373452000	1.042320000
H	5.322840000	–0.923985000	1.960098000
C	3.711686000	0.910581000	–0.106946000
C	4.813113000	1.853779000	–0.183682000
C	6.285044000	1.544706000	–0.243138000
H	6.828735000	2.442800000	–0.527405000
H	6.487611000	0.752797000	–0.962383000
H	6.636269000	1.214086000	0.734233000
C	4.255956000	3.105625000	–0.190120000
C	4.953357000	4.439834000	–0.220220000
H	4.271286000	5.190204000	–0.617760000
H	5.805369000	4.388198000	–0.896182000
C	5.427885000	4.855112000	1.187902000
H	4.578793000	4.915748000	1.868714000
H	5.919940000	5.826005000	1.148836000
H	6.130217000	4.116991000	1.575323000
C	2.826212000	2.938964000	–0.113943000
C	1.808840000	4.037809000	–0.113327000
H	0.837201000	3.667941000	0.197281000
H	1.738204000	4.446448000	–1.123041000
H	2.140669000	4.828905000	0.557252000
N	–9.413925000	0.611264000	–0.038097000
O	–10.288401000	–0.216847000	–0.090840000
O	–9.616362000	1.798989000	0.016659000

*Coordinates of the geometry of isomer **ctc** of* **NBT** *optimized with the M06HF functional*

S	–4.367597000	–1.309415000	–0.096739000
F	0.475305000	1.512173000	1.145863000
F	0.394154000	1.579466000	–1.148613000
N	–3.996219000	1.250254000	0.062550000
N	1.220334000	–0.442852000	–0.082989000
N	2.547721000	1.670539000	–0.078537000
B	1.114747000	1.087594000	–0.040630000
C	–5.767481000	–0.281966000	–0.051192000
C	–7.109291000	–0.638608000	–0.091999000
H	–7.441938000	–1.662979000	–0.161258000
C	–8.010785000	0.404637000	–0.040349000
C	–7.652715000	1.753094000	0.048218000

H	–8.421363000	2.509114000	0.085465000
C	–6.315441000	2.084147000	0.086667000
H	–5.992430000	3.111973000	0.155364000
C	–5.363050000	1.059545000	0.036258000
C	–3.358716000	0.131304000	–0.001837000
C	–1.894992000	0.067916000	0.005842000
H	–1.417304000	1.030732000	0.093841000
C	–1.231279000	–1.089306000	–0.086616000
H	–1.803700000	–2.007196000	–0.160040000
C	0.204793000	–1.346554000	–0.087799000
C	0.739899000	–2.643184000	–0.079621000
C	–0.035156000	–3.937244000	–0.050122000
H	0.579230000	–4.721437000	–0.488978000
H	–0.926504000	–3.858000000	–0.671407000
C	–0.432365000	–4.330072000	1.388110000
H	0.459709000	–4.420861000	2.008105000
H	–0.964430000	–5.280612000	1.389591000
H	–1.075826000	–3.564175000	1.821723000
C	2.138283000	–2.520421000	–0.045353000
C	3.089091000	–3.694272000	0.008069000
H	2.584196000	–4.536316000	0.478263000
H	3.983823000	–3.460375000	0.579019000
H	3.390312000	–3.987171000	–0.998558000
C	2.409708000	–1.140837000	–0.066735000
C	3.665089000	–0.452617000	–0.094458000
C	4.928510000	–1.242251000	–0.117442000
C	5.359293000	–1.825768000	–1.305646000
H	4.774768000	–1.704832000	–2.207816000
C	6.544008000	–2.553405000	–1.321733000
H	6.886863000	–3.001126000	–2.243407000
C	7.283705000	–2.708193000	–0.152179000
H	8.201531000	–3.278528000	–0.166510000
C	6.844256000	–2.129255000	1.034794000
H	7.415073000	–2.250427000	1.943953000
C	5.665891000	–1.390834000	1.053437000
H	5.315978000	–0.933232000	1.969178000
C	3.724597000	0.908698000	–0.111236000
C	4.836663000	1.838710000	–0.198613000
C	6.304708000	1.512528000	–0.261610000
H	6.857729000	2.404413000	–0.547749000
H	6.496158000	0.718365000	–0.981487000
H	6.654892000	1.178103000	0.714800000
C	4.293927000	3.096580000	–0.212984000
C	5.007397000	4.421962000	–0.256498000
H	4.330419000	5.178917000	–0.649996000
H	5.851033000	4.356457000	–0.941692000
C	5.502349000	4.837437000	1.144454000
H	4.661550000	4.911588000	1.834061000
H	6.005864000	5.802012000	1.095696000
H	6.199680000	4.092532000	1.527771000
C	2.862295000	2.946957000	–0.130787000
C	1.857582000	4.057473000	–0.131719000
H	0.882401000	3.699847000	0.182187000
H	1.789414000	4.463825000	–1.142493000
H	2.200108000	4.846672000	0.535787000

N	–9.439513000	0.069578000	–0.078507000
O	–10.235354000	0.973969000	–0.036326000
O	–9.747828000	–1.093870000	–0.150078000

*Coordinates of the geometry of isomer **ttt** of* **NBT** *optimized with the M06HF functional*

S	–4.937795000	–1.928485000	0.532455000
F	0.396989000	1.485620000	1.102949000
F	0.396317000	1.645607000	–1.182107000
N	–3.819059000	0.242496000	–0.320719000
N	1.256737000	–0.387913000	–0.166099000
N	2.522370000	1.745415000	–0.040325000
B	1.100412000	1.135846000	–0.069332000
C	–5.962345000	–0.578546000	0.163987000
C	–7.345270000	–0.478475000	0.259802000
H	–7.968163000	–1.293233000	0.595862000
C	–7.887385000	0.736408000	–0.102400000
C	–7.139847000	1.832710000	–0.546344000
H	–7.642132000	2.750026000	–0.809562000
C	–5.771152000	1.711768000	–0.637004000
H	–5.156459000	2.532307000	–0.974950000
C	–5.172558000	0.496380000	–0.279508000
C	–3.552857000	–0.956984000	0.068402000
C	–2.209380000	–1.544690000	0.150094000
H	–2.144371000	–2.557892000	0.515729000
C	–1.139203000	–0.819940000	–0.190566000
H	–1.293844000	0.204897000	–0.505607000
C	0.243740000	–1.288384000	–0.169905000
C	0.780456000	–2.587073000	–0.184996000
C	0.023817000	–3.890276000	–0.225032000
H	0.598625000	–4.611356000	–0.804402000
H	–0.919145000	–3.746693000	–0.750605000
C	–0.226990000	–4.457667000	1.188650000
H	0.724049000	–4.665496000	1.678377000
H	–0.802498000	–5.381174000	1.131603000
H	–0.768742000	–3.739527000	1.804138000
C	2.179045000	–2.453248000	–0.169707000
C	3.149555000	–3.611219000	–0.180192000
H	2.627423000	–4.518388000	0.115990000
H	3.975143000	–3.441184000	0.508016000
H	3.562502000	–3.756235000	–1.178800000
C	2.448627000	–1.070518000	–0.159512000
C	3.686923000	–0.359706000	–0.131611000
C	4.964236000	–1.126542000	–0.156295000
C	5.430100000	–1.657179000	–1.356249000
H	4.863264000	–1.509652000	–2.265714000
C	6.627216000	–2.364054000	–1.374390000
H	6.997530000	–2.770019000	–2.305107000
C	7.344732000	–2.551081000	–0.195627000
H	8.272345000	–3.105067000	–0.211714000
C	6.869896000	–2.026045000	1.002987000
H	7.423584000	–2.173133000	1.918865000
C	5.678669000	–1.308609000	1.024237000
H	5.301340000	–0.892088000	1.948975000
C	3.714828000	1.005036000	–0.082843000
C	4.809131000	1.956386000	–0.104681000

C	6.284280000	1.658472000	–0.146781000
H	6.826113000	2.564186000	–0.409473000
H	6.503584000	0.878043000	–0.873516000
H	6.622903000	1.316410000	0.831215000
C	4.243954000	3.205883000	–0.077132000
C	4.934157000	4.543930000	–0.047280000
H	4.259348000	5.302862000	–0.440878000
H	5.805406000	4.517385000	–0.699991000
C	5.366708000	4.917400000	1.385762000
H	4.497766000	4.953252000	2.043145000
H	5.855391000	5.890665000	1.392050000
H	6.060660000	4.169742000	1.769893000
C	2.816569000	3.028917000	–0.031708000
C	1.788708000	4.118124000	–0.010128000
H	0.820112000	3.730626000	0.289416000
H	1.715153000	4.547887000	–1.010855000
H	2.109497000	4.897694000	0.678843000
N	–9.345038000	0.882739000	–0.016653000
O	–9.825354000	1.950449000	–0.304526000
O	–9.991989000	–0.071146000	0.337182000

*Coordinates of the geometry of isomer **ttc** of* **NBT** *optimized with the M06HF functional*

S	–3.947283000	0.518655000	–0.486232000
F	0.341746000	1.452796000	1.071332000
F	0.371107000	1.599109000	–1.212942000
N	–4.581885000	–1.798904000	0.481301000
N	1.247701000	–0.414716000	–0.174219000
N	2.481537000	1.735645000	–0.042771000
B	1.069486000	1.106777000	–0.087443000
C	–5.623543000	0.200532000	–0.163826000
C	–6.718673000	1.034570000	–0.351844000
H	–6.630462000	2.035657000	–0.745421000
C	–7.943648000	0.505790000	–0.001966000
C	–8.130189000	–0.781709000	0.510661000
H	–9.123612000	–1.119926000	0.759199000
C	–7.029830000	–1.592240000	0.688723000
H	–7.128308000	–2.592438000	1.082798000
C	–5.764767000	–1.098419000	0.350112000
C	–3.572097000	–1.097271000	0.095769000
C	–2.199361000	–1.607180000	0.152974000
H	–2.120963000	–2.610691000	0.542996000
C	–1.141996000	–0.876923000	–0.211451000
H	–1.283610000	0.142429000	–0.553337000
C	0.247323000	–1.328503000	–0.182813000
C	0.799518000	–2.619787000	–0.192350000
C	0.059855000	–3.932642000	–0.235611000
H	0.640401000	–4.641875000	–0.823986000
H	–0.889026000	–3.797790000	–0.752864000
C	–0.174321000	–4.513096000	1.175616000
H	0.782103000	–4.706999000	1.660697000
H	–0.733421000	–5.446256000	1.114347000
H	–0.727327000	–3.808975000	1.797273000
C	2.196765000	–2.467417000	–0.169753000
C	3.181895000	–3.612853000	–0.176934000
H	2.668929000	–4.527608000	0.111517000

H	4.000281000	–3.435252000	0.517984000
H	3.603875000	–3.748615000	–1.173088000
C	2.448351000	–1.081788000	–0.159201000
C	3.676505000	–0.353564000	–0.122376000
C	4.963945000	–1.103497000	–0.139356000
C	5.444894000	–1.622776000	–1.338471000
H	4.882806000	–1.477713000	–2.251253000
C	6.650155000	–2.315620000	–1.351273000
H	7.031721000	–2.713049000	–2.281179000
C	7.361319000	–2.499754000	–0.168179000
H	8.295181000	–3.043105000	–0.180006000
C	6.871543000	–1.985976000	1.029392000
H	7.420458000	–2.130793000	1.948493000
C	5.671903000	–1.282550000	1.045515000
H	5.283133000	–0.875039000	1.969573000
C	3.684585000	1.011375000	–0.073371000
C	4.765827000	1.977919000	–0.085495000
C	6.245030000	1.698772000	–0.110969000
H	6.778492000	2.609905000	–0.371579000
H	6.481808000	0.917716000	–0.831487000
H	6.577095000	1.364918000	0.872126000
C	4.183449000	3.219643000	–0.064758000
C	4.853508000	4.567700000	–0.028893000
H	4.174871000	5.314853000	–0.438454000
H	5.737062000	4.550913000	–0.665186000
C	5.253743000	4.954641000	1.410085000
H	4.372411000	4.979742000	2.051395000
H	5.726468000	5.935717000	1.420364000
H	5.952468000	4.219957000	1.810352000
C	2.758399000	3.023170000	–0.033770000
C	1.715389000	4.097841000	–0.026576000
H	0.747538000	3.695979000	0.255736000
H	1.652675000	4.528738000	–1.027553000
H	2.013627000	4.880411000	0.669042000
N	–9.127018000	1.355818000	–0.181215000
O	–10.194788000	0.920726000	0.169719000
O	–8.973769000	2.447332000	–0.669271000

Table S2. Relative electronic energies of the four conformational isomers of **BT** with a *trans* configuration for their central [C=C] bond optimized with the restricted B3LYP and M06HF functionals and the corresponding values computed with single-point MP2 calculations [*a*].

Isomer	B3LYP (kcal mol^{-1})	B3LYP//MP2 (kcal mol^{-1})	M06HF (kcal mol^{-1})	M06HF//MP2 (kcal mol^{-1})
ctt	1.13	5.57	1.22	2.23
ctc	1.15	1.31	1.21	2.00
ttt	0.36	0.66	0.39	0.77
ttc	0	0	0	0

[*a*] Calculations were performed with the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN.

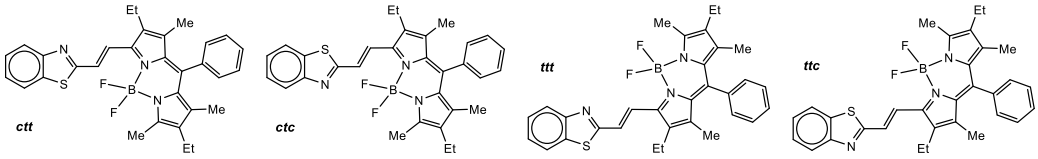


Table S3. Relative electronic energies of the four conformational isomers of **NBT** with a *trans* configuration for their central [C=C] bond optimized with the restricted B3LYP and M06HF functionals and the corresponding values computed with single-point MP2 calculations [*a*].

Isomer	B3LYP (kcal mol^{-1})	B3LYP//MP2 (kcal mol^{-1})	M06HF (kcal mol^{-1})	M06HF//MP2 (kcal mol^{-1})
ctt	0.79	1.62	1.00	1.91
ctc	1.09	1.24	1.33	1.68
ttt	0.14	0.78	0.23	0.62
ttc	0	0	0	0

[*a*] Calculations were performed with the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN.

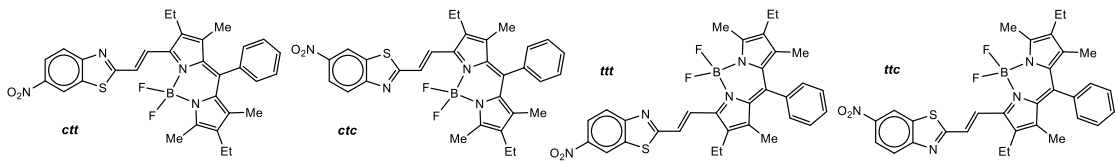


Table S4. Relative free energy (ΔG) of the four conformational isomers of **BT** with a *trans* configuration for their central [C=C] bond as well as vertical energy (ΔE), wavelength (λ), oscillator strength (f) and main orbital pair with its contribution for electronic transitions from the ground state to the corresponding first singlet excited state computed with the restricted B3LYP and M06HF functionals [*a*].

Functional	*Isomer*	ΔG (kcal mol^{-1})	ΔE (eV)	λ (nm)	f	*Main Orbital Pair*	*Contribution* (%)
B3LYP							
	ctt	1.21	2.20	564	1.0376	[HOMO] → [LUMO]	100
	ctc	1.12	2.21	561	1.0177	[HOMO] → [LUMO]	100
	ttt	0.36	2.27	546	1.0966	[HOMO] → [LUMO]	99
	ttc	0	2.29	542	1.1186	[HOMO] → [LUMO]	99
M06HF							
	ctt	3.42	2.60	476	0.7667	[HOMO] → [LUMO]	91
	ctc	2.74	2.58	480	0.7936	[HOMO] → [LUMO]	91
	ttt	0.69	2.64	471	0.8623	[HOMO] → [LUMO]	91
	ttc	0	2.65	467	0.8687	[HOMO] → [LUMO]	91

[*a*] The thermodynamic and photophysical parameters were computed with the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN at 25 °C.

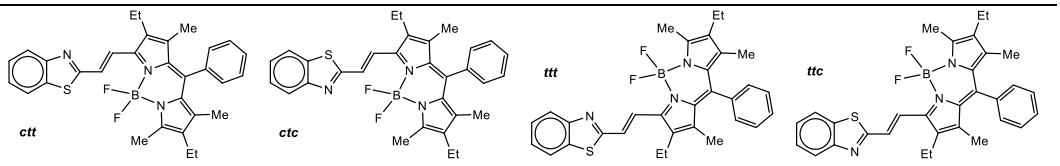
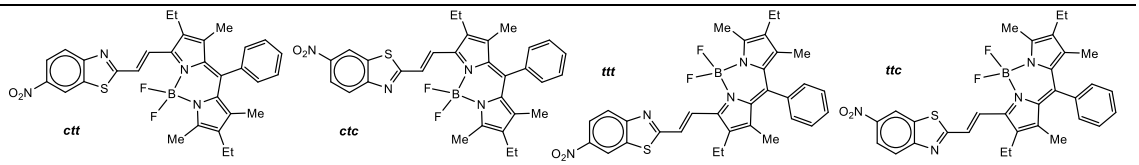


Table S5. Relative free energy (ΔG) of the four conformational isomers of **NBT** with a *trans* configuration for their central [C=C] bond as well as vertical energy (ΔE), wavelength (λ), oscillator strength (f) and main orbital pair with its contribution for electronic transitions from the ground state to the corresponding first singlet excited state computed with the restricted B3LYP and M06HF functionals [*a*].

Functional	*Isomer*	ΔG (kcal mol^{-1})	ΔE (eV)	λ (nm)	f	*Main Orbital Pair*	*Contribution* (%)
B3LYP							
	ctt	0.52	2.03	601	1.1610	[HOMO] → [LUMO]	100
	ctc	0.99	2.05	604	1.1348	[HOMO] → [LUMO]	100
	ttt	0.24	2.10	591	1.1430	[HOMO] → [LUMO]	99
	ttc	0	2.09	594	1.06	[HOMO] → [LUMO]	99
M06HF							
	ctt	1.21	2.60	477	0.8297	[HOMO] → [LUMO]	90
	ctc	2.43	2.62	473	0.8174	[HOMO] → [LUMO]	89
	ttt	0	2.65	467	0.8973	[HOMO] → [LUMO]	89
	ttc	1.32	2.67	464	0.8904	[HOMO] → [LUMO]	88

[*a*] The thermodynamic and photophysical parameters were computed with the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN at 25 °C.



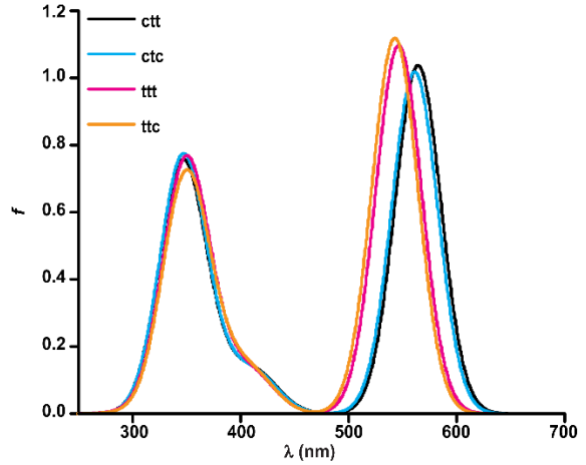


Figure S5. Absorption spectra of the four isomers of **BT** computed with the restricted B3LYP functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN and plotted with Gaussian broadening with a width at half maximum of 50 nm.

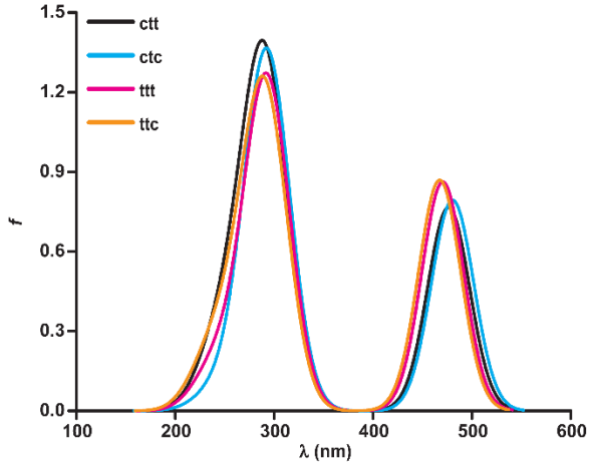


Figure S6. Absorption spectra of the four isomers of **BT** computed with the restricted M06HF functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN and plotted with Gaussian broadening with a width at half maximum of 50 nm.

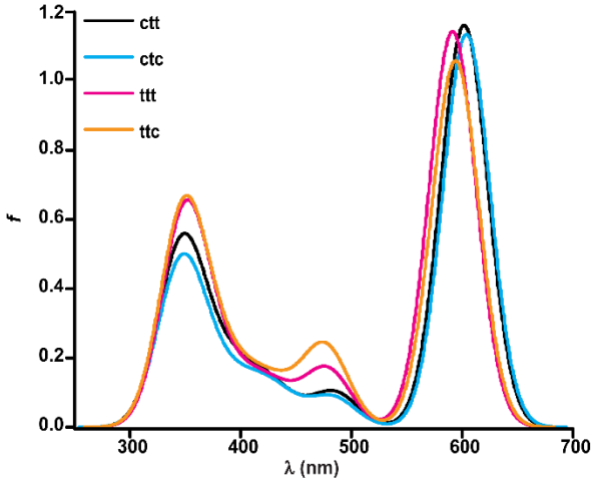


Figure S7. Absorption spectra of the four isomers of **NBT** computed with the restricted B3LYP functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN and plotted with Gaussian broadening with a width at half maximum of 50 nm.

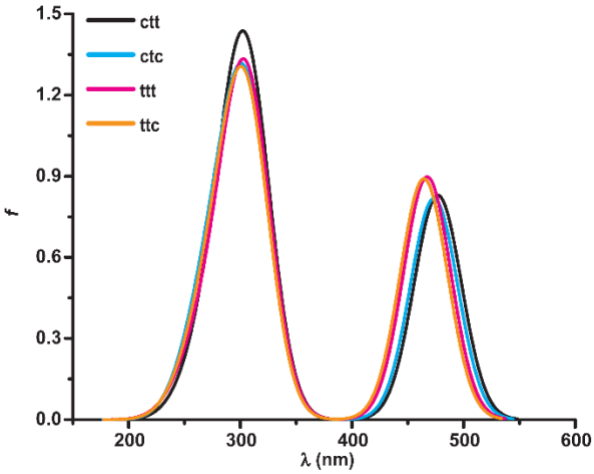
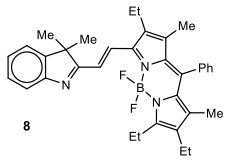


Figure S8. Absorption spectra of the four isomers of **NBT** computed with the restricted M06HF functional, the 6-311+G(d,p) basis set and the IEFPCM solvation model for MeCN and plotted with Gaussian broadening with a width at half maximum of 50 nm.

Table S6. Absorption (λ_{Ab}) and emission (λ_{Em}) wavelengths, fluorescence quantum yield (ϕ), molar absorption coefficient (ε) and brightness ($\phi \times \varepsilon$) of **BO**, **BT** and **NBT** in MeCN at 25 °C [*a*].

	λ_{Ab} (nm)	λ_{Em} (nm)	ϕ	ε ($mM^{-1}\,cm^{-1}$)	$\phi \times \varepsilon$ ($mM^{-1}\,cm^{-1}$)
BO	578	593	0.83	104	86
BT	584	597	0.85	124	105
NBT	592	613	0.44	120	53

[*a*] The values of ϕ were determined in aerated solutions against a MeCN solution of **8** (ϕ= 0.50).



8

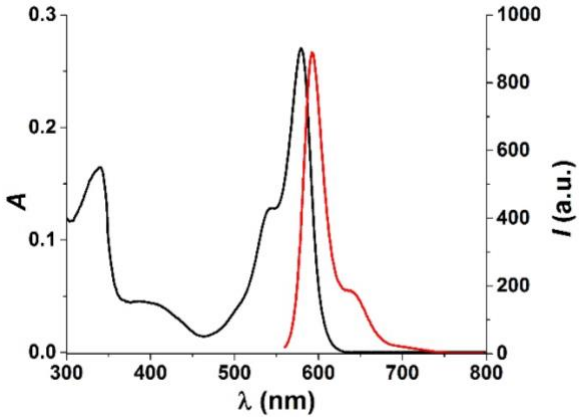


Figure S9. Absorption and emission (λ_{Ex} = 550 nm) spectra of **BO** (2.5 μM) in MeCN at 25 °C.

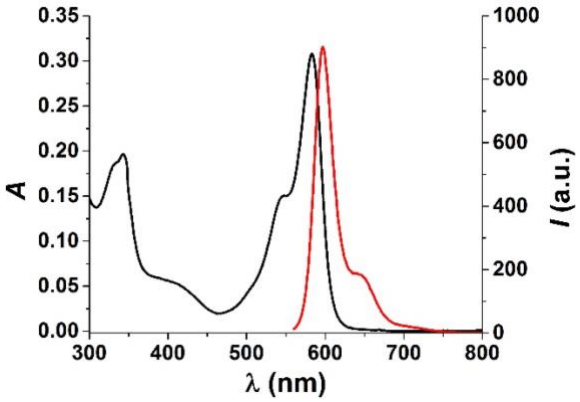


Figure S10. Absorption and emission (λ_{Ex} = 550 nm) spectra of **BT** (2.5 μM) in MeCN at 25 °C.

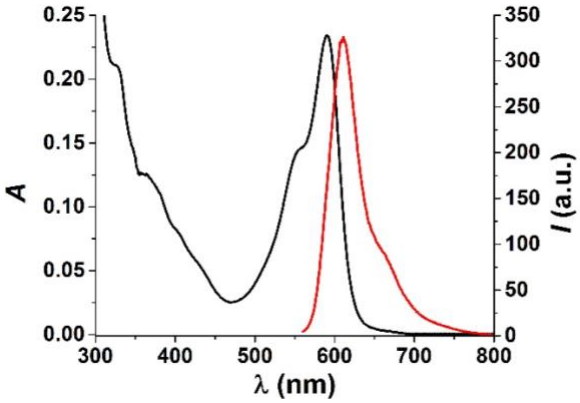


Figure S11. Absorption and emission (λ_{Ex} = 560 nm) spectra of **NBT** (2 μM) in MeCN at 25 °C.

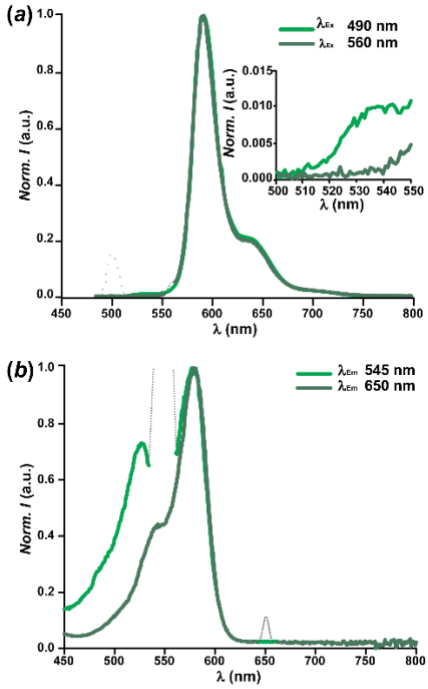


Figure S12. Normalized emission (**A**) and excitation (**B**) spectra of **BO** in MeCN at 25 °C.

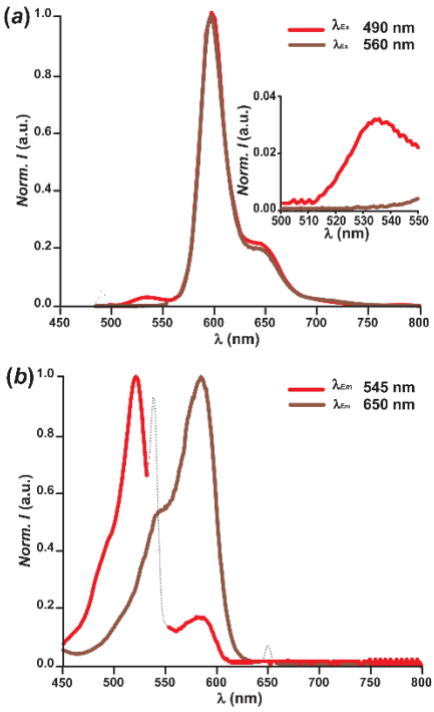


Figure S13. Normalized emission (**A**) and excitation (**B**) spectra of **BT** in MeCN at 25 °C.

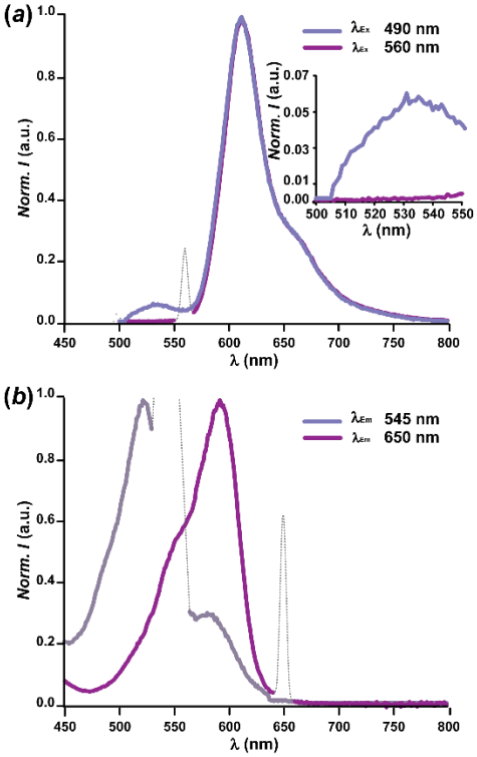


Figure S14. Normalized emission (**A**) and excitation (**B**) spectra of **NBT** in MeCN at 25 °C.

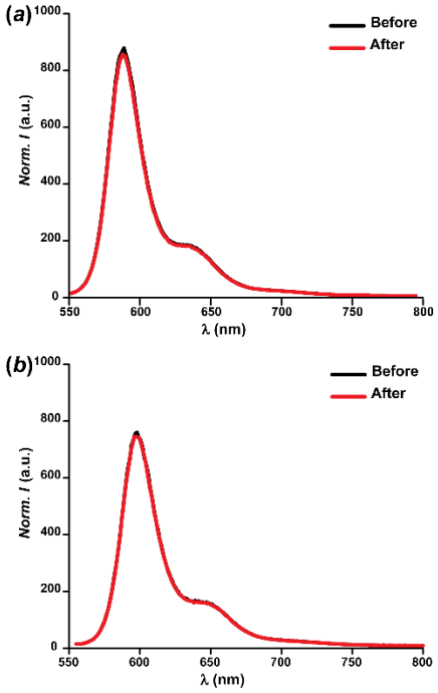


Figure S15. Emission spectra (λ_{Ex} = 550 nm) of **BO** in MeCN (6 µM) recorded before and after irradiation at either (**A**) 300–410 nm (3.70 mW cm^{-2}) or (**B**) 500–530 nm (0.18 mW cm^{-2}) for 240 s at 25 °C.

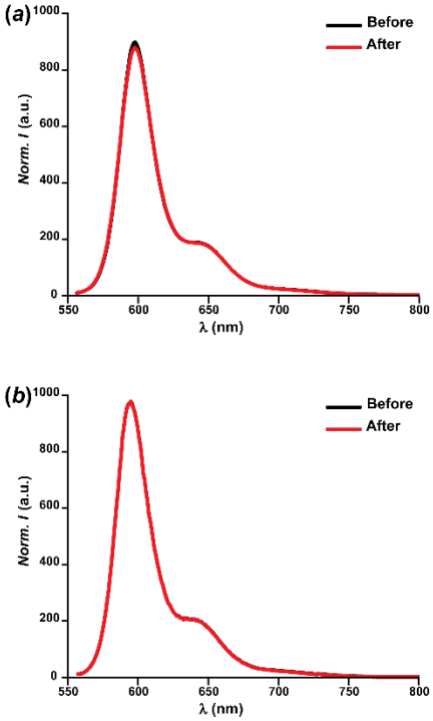


Figure S16. Emission spectra (λ_{Ex} = 550 nm) of **BT** in MeCN (5 µM) recorded before and after irradiation at either (**A**) 300–410 nm (3.70 mW cm^{-2}) or (**B**) 500–530 nm (0.18 mW cm^{-2}) for 240 s at 25 °C.

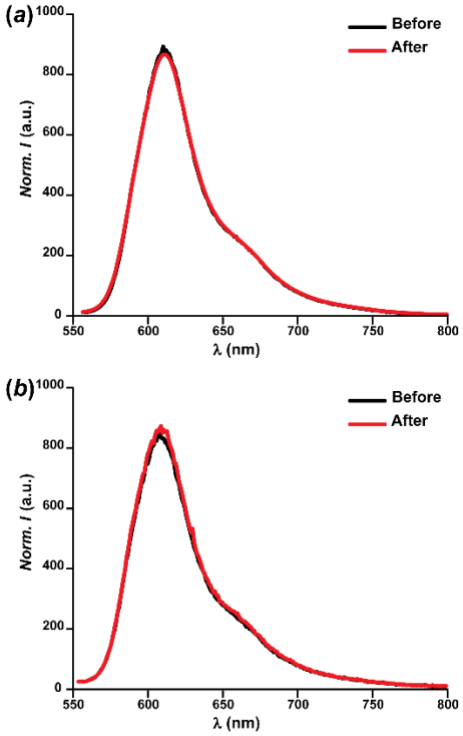


Figure S17. Emission spectra (λ_{Ex} = 550 nm) of **NBT** in MeCN (6 or 3 µM) recorded before and after irradiation at either (**A**) 300–410 nm (3.70 mW cm^{-2}) or (**B**) 500–530 nm (0.18 mW cm^{-2}) for 240 s at 25 °C.

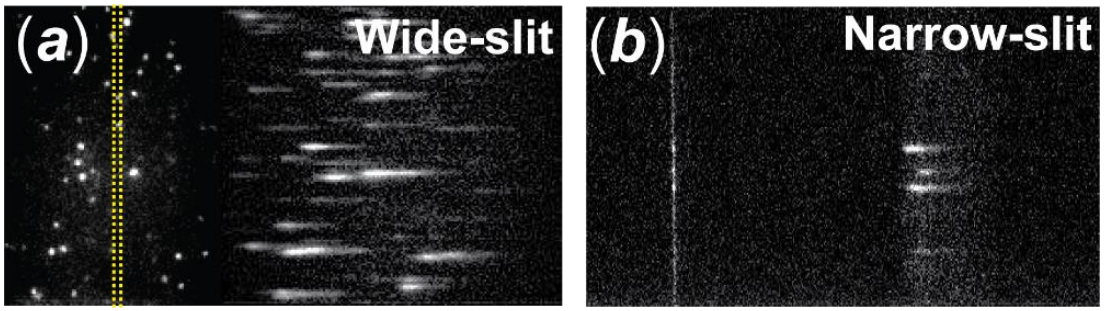


Figure S18. Raw images of (***a***) wide-slit and (***b***) narrow-slit configurations with 5 mm and 50 μm entrance slit widths respectively. Yellow dashed box in (***a***) indicates the adjustment of entrance slit width and the confinement of FOV to minimize the detection of multiple single molecules with overlapping spectra along similar horizontal coordinate.

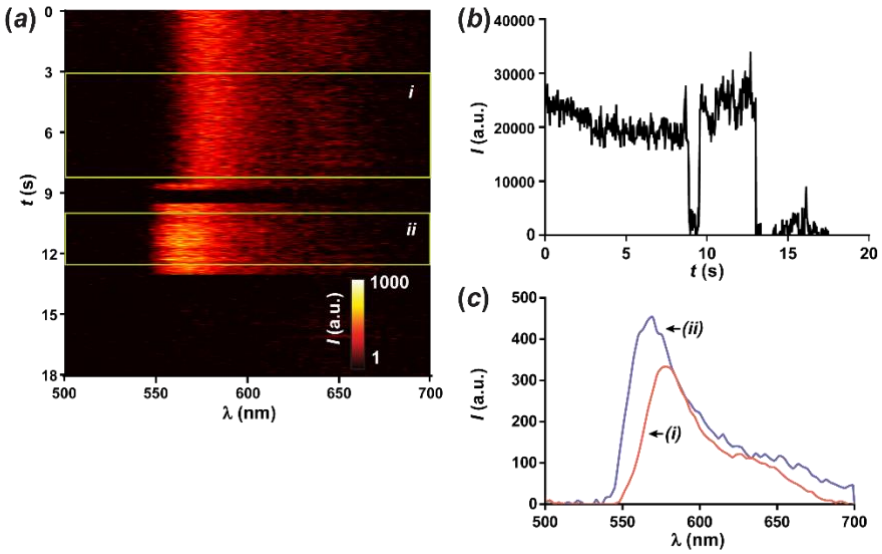


Figure S19. Emission spectra (***a***) and intensity evolutions (***b***) of a single **BO** molecule together with the averaged emission spectra (***c***) from 3.2–8.8 s (***i***) and 10.3–12.4 s (***ii***) of the acquisition duration.

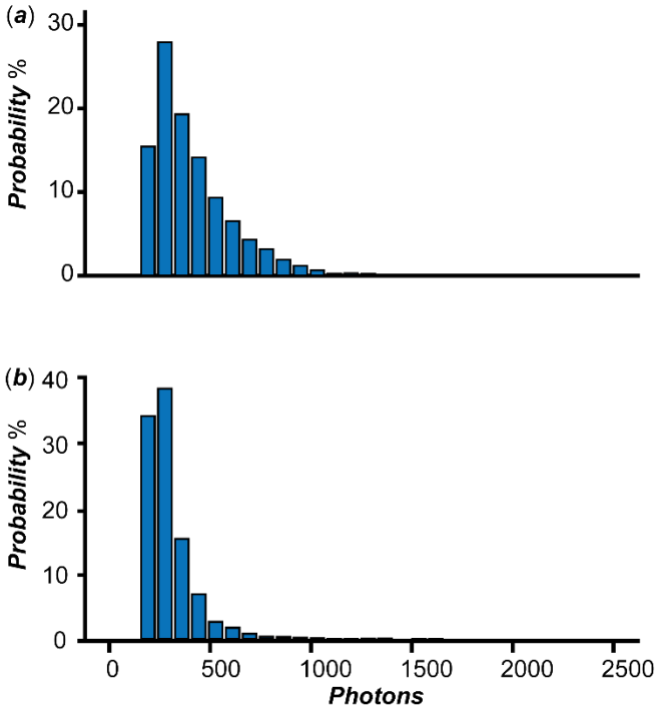


Figure S20. Histograms of photon distributions of **BO** single molecules in the spectral window of 550-600 nm ***(a)*** and 600-650 nm (***b***).

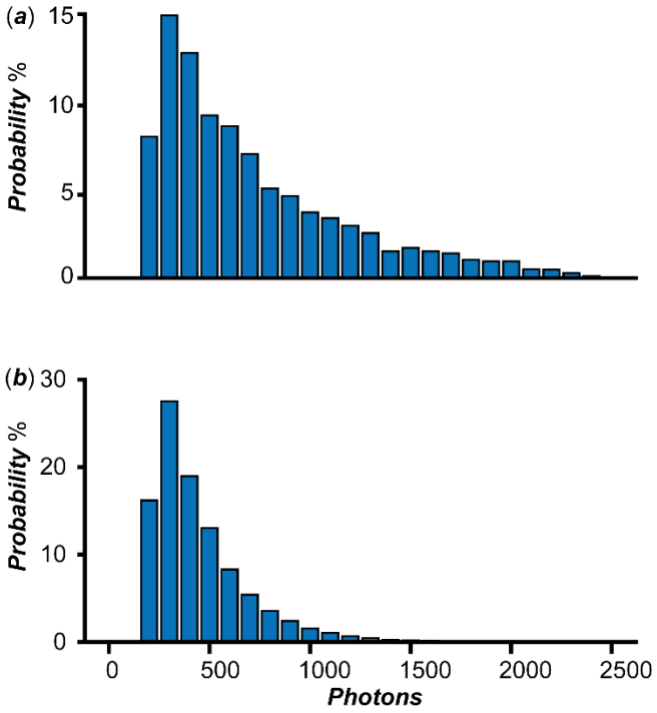


Figure S21. Histograms of photon distributions of **BT** single molecules in the spectral window of 550-600 nm (***a***) and 600-650 nm (***b***).

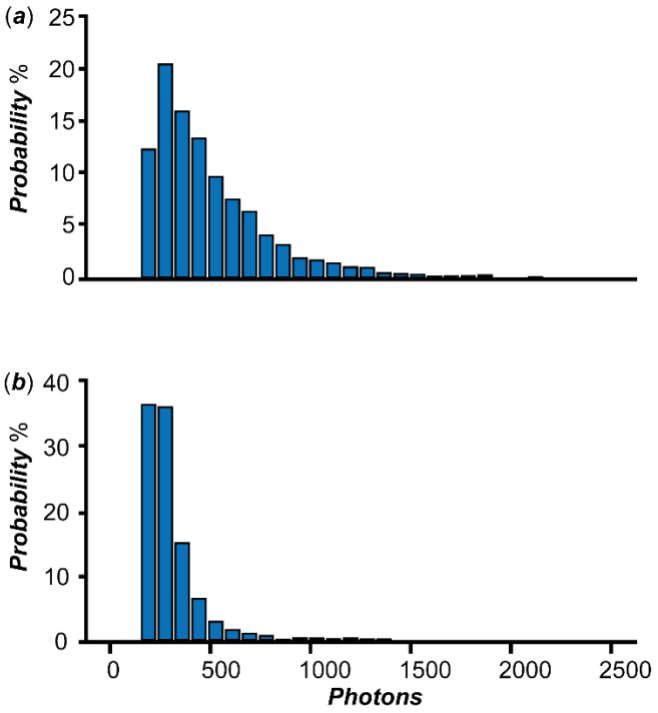


Figure S22. Histograms of photon distributions of **NBT** single molecules in the spectral window of 550-600 nm (***a***) and 600-650 nm ***(b)***.

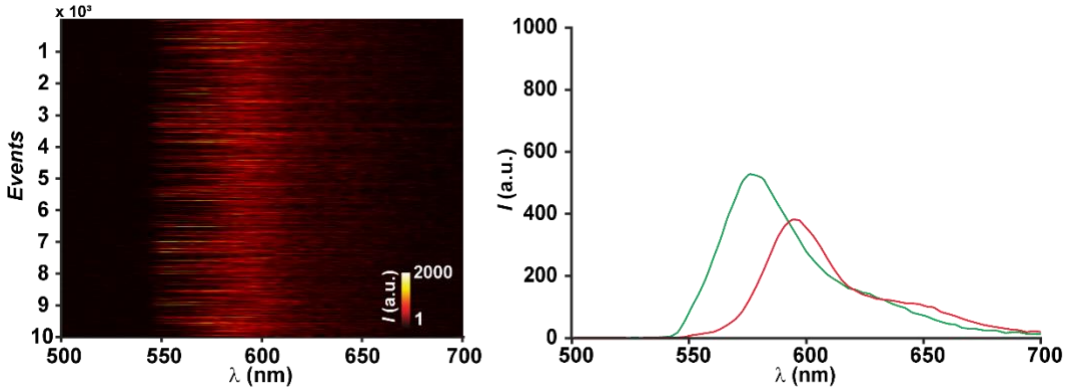


Figure S23. 10,052 single-molecule emission spectra of **BO** and the averaged emission spectra extracted from the molecules with spectral centroid of 590–596 nm (green line) and 611–617 nm (red line).

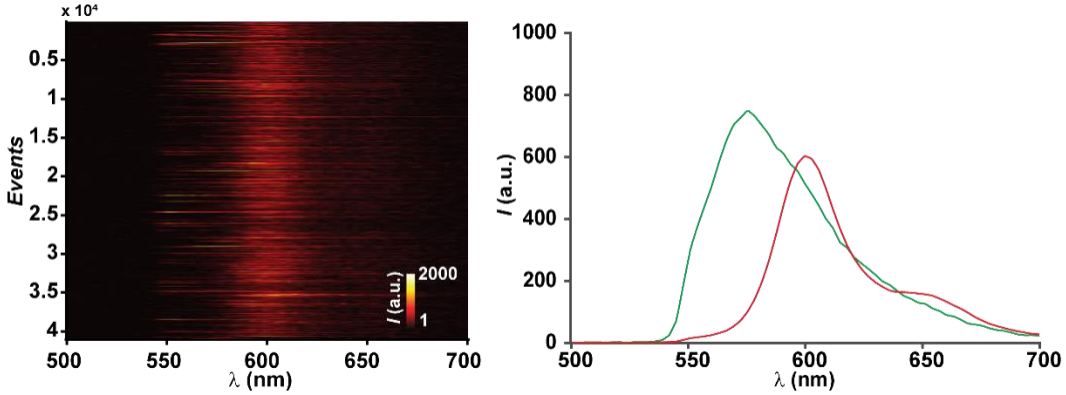


Figure S24. 40,949 single-molecule emission spectra of **BT** and the averaged emission spectra extracted from the molecules with spectral centroid of 590–596 nm (green line) and 611–617 nm (red line).

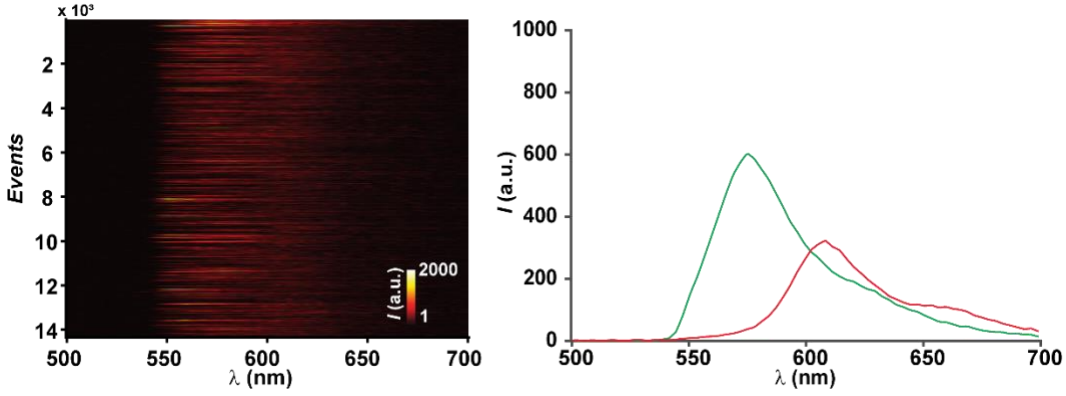


Figure S25. 14,349 single-molecule emission spectra of **NBT** and the averaged emission spectra extracted from the molecules with spectral centroid of 590–596 nm (green line) and 620–626 nm (red line).