**Supporting Information for**

**Organic Thermally Activated Delayed Fluorescence Material with Strained Benzoguanidine Donor**

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Figure S1. 1H NMR (DMSO-d6) spectrum of **4BGIPN**.

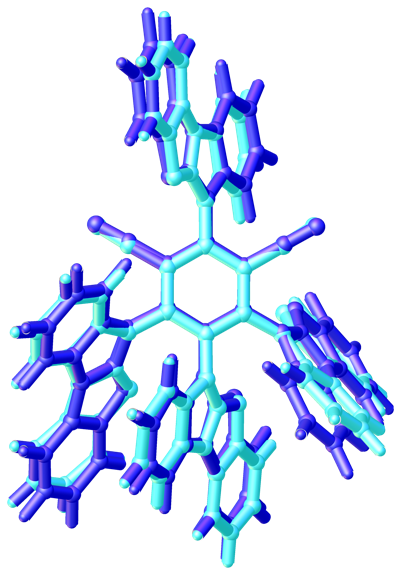
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Figure S2. 13C NMR (DCM-d2) spectrum of **4BGIPN**



**Figure S1.** Thermogravimetric analysis for compound **4BGIPN**.



**Figure S2.** An overlay of the X-ray crystal structure and optimised S0 geometry of compound **4BGIPN**.

**Photophysical Characterisation.**

UV-visible absorption spectra were recorded using a Varian Cary 5000 UV-Vis-NIR spectrometer. Photoluminescence measurements were recorded on an Edinburgh Instruments FLS980 spectrometer with a solids mount attachment where appropriate. Absolute photoluminescence quantum yields were recorded using Hamamatsu Quantaurus-QY C11347-11. Quantum yields have been measured in air for solid samples and under nitrogen for solutions. Time resolved luminescence data were collected on a time-correlated single photon counting (TCSPC) Edinburgh Instruments FLS980 spectrometer using F-900 software. A xenon flash lamp and EPL pulsed diode lasers were used as excitation sources. The collected data were analysed using F-900 software.

**Computational Details.**

**Table S1.** HOMO and LUMO molecular orbitals in crystal and optimized S0 geometry.

|  |  |  |
| --- | --- | --- |
|  | HOMO | LUMO |
| (crystal)  Overlap integral: 0.27 |  |  |
| (opt)  Overlap integral: 0.29 | A picture containing fruit, vegetable  Description automatically generated |  |

**Tables S2.** Dipole moments in S0 and S1 states in crystal and optimized S0 geometry.

|  |  |  |
| --- | --- | --- |
|  | S0 | S1 |
| (crystal) | 6.7D | 13.6D |
| (opt) | 6.4D | 7.2D |

**Table S3.** Vertical excitations S0 → S1 and S0→ Tn, character and oscillator strength coefficients for S0 → S1 in crystal and optimized S0 geometry.

|  |  |  |  |
| --- | --- | --- | --- |
|  | Excitation energy | Character | Oscillator strength |
| (crystal) | S1: 3.11eV = 399nm | HOMO – LUMO (92%) | 0.0773 |
| T1: 2.94eV = 422nm | HOMO – LUMO (71%) |  |
| T2: 3.09eV = 402nm | HOMO-2 – LUMO (19%)  HOMO-1 – LUMO (19%) |  |
| T3: 3.13eV = 396nm | HOMO-2 – LUMO (47%) |  |
| (opt) | S1: 3.19eV = 388nm | HOMO – LUMO (78%) | 0.0906 |
| T1: 2.99eV = 415nm | HOMO – LUMO (46%)  HOMO-1 – LUMO (18%) |  |
| T2: 3.05eV = 406nm | HOMO – LUMO (35%)  HOMO-3 – LUMO (19%)  HOMO – LUMO+1 (16%) |  |
| T3: 3.18eV = 389nm | HOMO-1 – LUMO (50%)  HOMO – LUMO+1 (31%) |  |

**Table S4.** HONTO and LUNTO molecular orbitals of the excited states in crystal and optimized S0 geometry.

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | HONTO | LUNTO |
| (crystal) | S1 | A picture containing outdoor object  Description automatically generated |  |
| T1 |  | A close-up of a necklace  Description automatically generated with low confidence |
| T2 | A picture containing arrow  Description automatically generated |  |
| T3 | A close-up of a tree branch with red berries  Description automatically generated with low confidence | A close-up of a necklace  Description automatically generated with low confidence |
| (opt) | S1 | A picture containing fruit  Description automatically generated |  |
| T1 | A picture containing fruit  Description automatically generated |  |
| T2 | Chart  Description automatically generated with medium confidence |  |
| T3 | A picture containing fruit  Description automatically generated |  |

**Coordinates for compound 4BGIPN in the ground state S0 geometry (crystal geometry).**

N 14.31500000 9.19000000 7.14100000

N 10.55200000 13.38100000 7.44200000

N 9.72700000 10.69700000 6.79700000

N 7.74300000 9.98600000 7.53600000

N 9.48500000 9.18400000 8.75300000

N 8.82600000 12.44200000 8.95700000

N 13.24800000 13.72600000 8.36300000

N 8.97500000 14.65100000 8.38400000

N 11.54000000 14.19500000 10.08800000

N 15.93700000 10.16600000 5.55500000

N 16.09200000 8.04800000 6.42700000

N 13.14800000 15.68000000 9.45200000

C 12.01500000 10.00100000 6.90600000

C 9.07200000 9.90900000 7.74300000

C 11.49300000 12.32100000 7.39700000

N 16.02600000 11.63900000 8.94600000

C 7.15400000 9.27800000 8.56500000

C 11.08200000 11.03100000 7.01200000

C 12.82500000 12.50700000 7.81300000

C 8.74500000 11.32800000 6.02600000

N 11.31800000 7.70900000 5.92100000

C 9.45200000 13.37800000 8.28800000

C 12.56200000 14.45100000 9.32700000

C 13.35100000 10.20600000 7.26800000

C 15.01900000 11.56300000 8.37900000

C 8.24900000 8.78500000 9.30700000

C 13.73100000 11.46500000 7.76200000

C 11.60400000 8.73400000 6.34900000

C 15.43700000 9.28700000 6.34200000

C 7.49200000 10.84800000 6.48100000

C 14.26900000 14.57500000 7.86000000

C 10.76800000 14.72000000 7.04200000

C 7.82000000 13.17900000 9.59500000

C 14.28400000 7.90200000 7.71400000

C 9.81600000 15.52700000 7.66900000

C 6.83300000 12.72200000 10.44800000

H 6.75900000 11.80200000 10.67300000

C 8.02300000 7.99700000 10.42100000

H 8.74900000 7.65100000 10.92700000

C 7.89100000 14.55400000 9.26500000

C 8.84000000 12.17900000 4.93900000

H 9.67800000 12.51600000 4.64300000

C 11.70800000 15.27000000 6.19400000

H 12.34200000 14.72800000 5.73800000

C 15.37400000 7.20800000 7.27000000

C 5.66100000 8.20200000 10.03500000

H 4.77700000 7.98400000 10.30800000

C 11.39700000 15.40800000 10.79100000

C 14.21200000 15.80400000 8.52200000

C 6.33500000 11.19100000 5.82400000

H 5.48900000 10.86900000 6.11500000

C 17.04200000 9.45900000 5.01400000

C 6.44300000 12.03000000 4.71300000

H 5.65700000 12.26300000 4.23300000

C 15.18900000 14.36900000 6.82800000

H 15.25300000 13.54100000 6.36600000

C 5.94800000 13.66700000 10.96200000

H 5.27300000 13.38000000 11.56600000

C 7.03500000 15.49100000 9.77600000

H 7.11900000 16.41600000 9.57300000

C 5.84200000 8.98400000 8.91200000

H 5.10700000 9.30400000 8.40300000

C 6.73000000 7.72600000 10.77700000

H 6.56100000 7.20000000 11.55000000

C 17.15000000 8.16300000 5.53400000

C 6.01300000 14.99400000 10.62700000

H 5.36300000 15.59400000 10.97400000

C 9.78200000 16.87200000 7.50600000

H 9.12600000 17.40500000 7.93900000

C 7.64200000 12.52100000 4.29800000

H 7.66800000 13.11100000 3.55400000

C 10.46100000 15.76700000 11.74600000

H 9.78000000 15.16100000 12.01200000

C 15.63300000 5.86600000 7.66900000

H 16.37400000 5.36100000 7.35600000

C 12.39600000 16.34100000 10.41600000

C 11.68500000 16.64200000 6.03800000

H 12.33000000 17.05600000 5.47800000

C 10.74100000 17.43200000 6.68300000

H 10.75400000 18.37400000 6.55700000

C 17.97100000 9.91300000 4.07800000

H 17.93800000 10.79500000 3.72300000

C 10.54300000 17.01500000 12.29700000

H 9.91800000 17.26000000 12.96700000

C 11.50000000 17.93100000 11.91500000

H 11.50000000 18.79900000 12.29800000

C 16.00200000 15.45300000 6.52400000

H 16.62900000 15.35800000 5.81600000

C 13.38000000 7.35200000 8.59900000

H 12.61700000 7.83300000 8.89900000

C 15.05200000 16.84200000 8.24400000

H 15.03200000 17.65400000 8.73600000

C 12.48100000 17.58700000 10.95800000

H 13.16600000 18.19500000 10.70600000

C 19.02100000 7.69900000 4.24000000

H 19.71000000 7.11400000 3.94400000

C 18.14500000 7.25200000 5.17000000

H 18.20300000 6.38300000 5.54700000

C 13.64700000 6.03800000 9.03500000

H 13.07500000 5.62500000 9.66900000

C 18.95600000 8.99100000 3.69600000

H 19.60000000 9.24900000 3.04600000

C 15.95000000 16.63600000 7.18100000

H 16.53200000 17.34100000 6.91800000

C 14.69900000 5.37300000 8.56000000

H 14.81900000 4.48000000 8.86200000

**Coordinates for compound 4BGIPN in the ground state S0 geometry (optimized geometry).**

N 3.83442600 0.90870300 -0.29780500

N -1.50230400 -0.52172100 0.65031500

N -0.54057900 2.03640200 1.38865100

N -2.02326100 3.70084800 1.16456000

N -0.36054800 3.76416300 -0.37286600

N -2.68040900 1.27132700 -0.57465100

N 0.28696900 -2.33182700 -0.65743800

N -3.70099500 -0.56708400 0.26534200

N -1.85021900 -1.91604700 -1.84132600

N 5.04490800 -1.00589500 0.69914400

N 6.05642500 0.74200300 -0.32996600

N -1.16351300 -3.95898100 -1.15101700

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C -0.85532500 3.18418900 0.66862000

C -0.15923300 -0.18673000 0.43780100

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C -2.37082900 4.72234800 0.29119800

C 0.30649200 1.07789400 0.81955000

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N 2.58001900 3.58120700 1.69188600

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C 4.90542300 0.11638500 0.06799500

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H 6.70389500 -3.02672900 1.76386700

C -4.95699500 -3.78448400 -2.67744200

H -5.95695300 -3.66472400 -3.07483800

C -4.54038000 -5.05383700 -2.25640400

H -5.22366100 -5.88954300 -2.33481300

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H 2.61715600 3.22133900 -1.49168400

C 0.09538300 -5.87842000 -0.07758800

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H 8.95627400 0.84241300 -0.48709400

C 4.49353900 4.11538500 -2.09254100

H 4.01753300 4.97679600 -2.54113600

C 8.57162100 -2.11033500 1.18471300

H 9.17877200 -2.90136800 1.60619100

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