Synthesis by a cost-effective method and electroluminescence of a novel efficient yellowish-green thermally-activated delayed fluorescent molecule

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**Figure S1**: $^1$H-NMR, $^{13}$C-NMR and $^{19}$F-NMR spectra of the 2,4,6-tris(4-fluorophenyl)-1,3,5-triazine (2).

**Figure S2**: $^1$H-NMR, $^{13}$C-NMR and FTIR spectra of the 2,4,6-tris(4-(10H-phenothiazin-10-yl)phenyl)-1,3,5-triazine (TRZ 3(Ph-PTZ)).

**Figure S3**: Advantage of the 2,4,6-tris(4-fluorophenyl)-1,3,5-triazine (2).

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Figure S1: $^1$H-NMR, $^{13}$C-NMR, $^{19}$F-NMR spectra of the 2,4,6-tris(4-fluorophenyl)-1,3,5-triazine (2).
**Figure S2:** $^1$H-NMR, $^{13}$C-NMR and FTIR spectra of the 2,4,6-tris(4-(10H-phenothiazin-10-yl)phenyl)-1,3,5-triazine (TRZ 3(Ph-PTZ)).
Figure S3: Advantage of the 2,4,6-tris(4-fluorophenyl)-1,3,5-triazine (2).

The S3 scheme shows that the 2,4,6-tris(4-fluorophenyl)-1,3,5-triazine enables us to synthesis with a simple reaction the molecule (1), (2), (3) or (4) (for respectively: 2,4,6-tri(4-carbazolephenyl)-1,3,5-triazine; 2,4,6-tri(4-phenoazinophenyl)-1,3,5-triazine; 2,4,6-tri(4-phenothiazinephenyl)-1,3,5-triazine; 2,4,6-tri(4-(9,9-dimethyl-9,10-dihydroacridine) phenyl)-1,3,5-triazine).
Figure S4: Energy diagram of the fabricated OLEDs with the HOMO and LUMO values (in eV) of each organic layer.
Figure S5: Reproducibility of the EL properties of the TADF OLEDs

| TRZ$_3$(Ph-PTZ):mCBP (6 wt.%) | EQE (%) |
|-------------------------------|---------|
| Device 1                      | 17.4    |
| Device 2                      | 16.8    |
| Device 3                      | 17.2    |
Table S1: B3LYP/6-31G(d) computed Cartesian coordinates of the conformers of 2,4,6-tris(4-(10H-phenothiazin-10-yl)phenyl)-1,3,5-triazine (TRZ 3(Ph-PTZ)).

**Conformer A-1**
Total energy: E(RB3LYP) = -3716.76685191 a.u.

| Center Number | Atomic Number | Coordinates (Angstroms) | X     | Y     | Z     |
|---------------|---------------|-------------------------|-------|-------|-------|
| 1             | 6             | -1.26543                | -0.355 | -0.37015 |
| 2             | 7             | -0.33958                | -1.32918 | -0.3705 |
| 3             | 6             | 0.939651                | -0.91837 | -0.36972 |
| 4             | 6             | 0.324565                | 1.272746 | -0.37016 |
| 5             | 7             | -0.98156                | 0.957751 | -0.37106 |
| 6             | 7             | 1.31992                 | 0.370269 | -0.37054 |
| 7             | 6             | -2.68607                | -0.75423 | -0.36972 |
| 8             | 6             | -3.06221                | -2.10559 | -0.36395 |
| 9             | 6             | -3.71032                | 0.204181 | -0.36326 |
| 10            | 6             | -4.39615                | -2.48742 | -0.37157 |
| 11            | 1             | -2.28701                | -2.86354 | -0.34708 |
| 12            | 6             | -5.04817                | -0.16369 | -0.37089 |
| 13            | 1             | -3.44262                | 1.254767 | -0.34591 |
| 14            | 6             | -5.42538                | -1.52286 | -0.39161 |
| 15            | 1             | -4.6374                 | -3.54223 | -0.34469 |
| 16            | 1             | -5.80294                | 0.611163 | -0.34326 |
| 17            | 6             | 1.995414                | -1.94919 | -0.36888 |
| 18            | 6             | 3.353689                | -1.59888 | -0.36296 |
| 19            | 6             | 1.677868                | -3.31552 | -0.3624 |
| 20            | 6             | 4.351601                | -2.56291 | -0.37063 |
| 21            | 1             | 3.622199                | -0.5485  | -0.34596 |
| 22            | 6             | 2.665658                | -4.28992 | -0.37003 |
| 23            | 1             | 0.634247                | -3.60922 | -0.34496 |
| 24            | 6             | 4.031253                | -3.93659 | -0.39087 |
| 25            | 1             | 5.385624                | -2.24416 | -0.3435 |
| 26            | 1             | 2.371964                | -5.33133 | -0.34249 |
| 27            | 6             | 0.689537                | 2.702425 | -0.36972 |
| 28            | 6             | 2.03166                 | 3.110288 | -0.36382 |
| 29            | 6             | -0.29277                | 3.703797 | -0.36333 |
| 30            | 6             | 2.381934                | 4.452848 | -0.37145 |
| 31            | 1             | 2.807647                | 2.353161 | -0.34675 |
| 32            | 6             | 0.043464                | 5.049953 | -0.37099 |
| 33            | 1             | -1.33675                | 3.411352 | -0.34599 |
| 34            | 6             | 1.393382                | 5.459055 | -0.39167 |
| 35            | 1             | 3.430739                | 4.718948 | -0.34433 |
| 36            | 1             | -0.74938                | 5.786271 | -0.34345 |
| 37            | 7             | 5.042501                | -4.92363 | -0.40689 |
|   |   |            |            |            |            |
|---|---|------------|------------|------------|------------|
| 38| 6 | 4.743777  | -6.31309  | -0.25631  |
| 39| 6 | 6.42441   | -4.59111  | -0.2575   |
| 40| 6 | 5.251195  | -7.00275  | 0.856677  |
| 41| 6 | 4.009521  | -7.01528  | -1.21937  |
| 42| 6 | 7.127046  | -5.08088  | 0.855297  |
| 43| 6 | 7.107902  | -3.84079  | -1.21162  |
| 44| 6 | 4.981697  | -8.36391  | 1.026467  |
| 45| 6 | 6.264683  | -6.11472  | 2.029454  |
| 46| 6 | 3.719938  | -8.36651  | -1.03507  |
| 47| 6 | 3.657861  | -6.48854  | -2.10095  |
| 48| 6 | 8.481408  | -4.77836  | 1.024014  |
| 49| 6 | 8.45184   | -3.51833  | -1.03854  |
| 50| 1 | 6.572146  | -3.50266  | -2.10308  |
| 51| 6 | 4.197575  | -9.03908  | 0.092427  |
| 52| 1 | 5.392338  | -8.88799  | 1.884764  |
| 53| 1 | 3.133477  | -8.89654  | -1.78002  |
| 54| 1 | 9.015956  | -5.17558  | 1.881995  |
| 55| 6 | 9.136654  | -3.97872  | 0.088743  |
| 56| 1 | 8.966903  | -2.91967  | -1.78429  |
| 57| 1 | 3.981252  | -10.0943  | 0.232793  |
| 58| 1 | 10.18638  | -3.73677  | 0.228147  |
| 59| 7 | 1.743084  | 6.828213  | -0.40746  |
| 60| 6 | 3.096124  | 7.263449  | -0.258    |
| 61| 6 | 0.764795  | 7.859086  | -0.25623  |
| 62| 6 | 3.441246  | 8.046825  | 0.855137  |
| 63| 6 | 4.070246  | 6.978733  | -1.22222  |
| 64| 6 | 0.839186  | 8.711496  | 0.857208  |
| 65| 6 | -0.22775  | 8.076998  | -1.21908  |
| 66| 6 | 4.755185  | 8.493312  | 1.023978  |
| 67| 16| 2.16695  | 8.480184  | 2.029679  |
| 68| 6 | 5.385636  | 7.402801  | -1.03904  |
| 69| 1 | 3.788753  | 6.411363  | -2.1038   |
| 70| 6 | -0.09945  | 9.733331  | 1.027823  |
| 71| 6 | -1.17839  | 9.079854  | -1.03411  |
| 72| 1 | -0.25393  | 7.444662  | -2.101    |
| 73| 6 | 5.730814  | 8.151929  | 0.088513  |
| 74| 1 | 5.004936  | 9.110339  | 1.882209  |
| 75| 1 | 6.136999  | 7.159942  | -1.78489  |
| 76| 1 | -0.02155  | 10.39412  | 1.886277  |
| 77| 6 | -1.12055  | 9.90212   | 0.093826  |
| 78| 1 | -1.95515  | 9.227504  | -1.77887  |
| 79| 1 | 6.753094  | 8.491632  | 0.227984  |
| 80| 1 | -1.85452  | 10.69037  | 0.234707  |
| 81| 7 | -6.78595  | -1.90454  | -0.40709  |
| 82| 6 | -7.83947  | -0.95049  | -0.25737  |
| 83| 6 | -7.18968  | -3.26725  | -0.25704  |
| 84| 6 | -8.69069  | -1.04396  | 0.855533  |
| 85| 6 | -8.07997  | 0.035842  | -1.2212   |
| Center Number | Atomic Number | X          | Y        | Z        |
|---------------|---------------|------------|----------|----------|
| 86            | 6             | -7.96551   | -3.62975 | 0.85589  |
| 87            | 6             | -6.88202   | -4.23511 | -1.2205  |
| 88            | 6             | -9.73441   | -0.12945 | 1.024683 |
| 89            | 16            | -8.42909   | -2.36501 | 2.029211 |
| 90            | 6             | -9.10502   | 0.962818 | -1.0377  |
| 91            | 1             | -7.44793   | 0.076088 | -2.1028  |
| 92            | 6             | -8.3815    | -4.95356 | 1.02537  |
| 93            | 6             | -7.27557   | -5.55987 | -1.03666 |
| 94            | 1             | -6.32102   | -3.9411  | -2.10207 |
| 95            | 6             | -9.9265    | 0.886621 | 0.089711 |
| 96            | 1             | -10.3938   | -0.22217 | 1.882766 |
| 97            | 1             | -9.27037   | 1.735245 | -1.78325 |
| 98            | 1             | -8.99307   | -5.21697 | 1.883423 |
| 99            | 6             | -8.01706   | -5.92163 | 0.090742 |
| 100           | 1             | -7.015     | -6.30585 | -1.78194 |
| 101           | 1             | -10.7319   | 1.602001 | 0.229435 |
| 102           | 1             | -8.33302   | -6.95142 | 0.230702 |

Conformer A-2
Total energy: \( E(RB3LYP) = -3716.76674964 \) a.u
|   |   |     |     |     |
|---|---|-----|-----|-----|
| 21 | 1 | -3.15215 | 1.837928 | -0.35948 |
| 22 | 6 | -0.88932 | 4.965548 | -0.2512 |
| 23 | 1 | 0.742038 | 3.586364 | -0.08705 |
| 24 | 6 | -2.28354 | 5.138553 | -0.37902 |
| 25 | 1 | -4.16433 | 4.062985 | -0.45955 |
| 26 | 1 | -0.23651 | 5.826403 | -0.18585 |
| 27 | 6 | -1.62199 | -2.26379 | -0.2372 |
| 28 | 6 | -3.01607 | -2.15086 | -0.34434 |
| 29 | 6 | -1.0785 | -3.5561 | -0.17815 |
| 30 | 6 | -3.83177 | -3.27138 | -0.40991 |
| 31 | 1 | -3.45961 | -1.16177 | -0.37027 |
| 32 | 6 | -1.88249 | -4.68461 | -0.24279 |
| 33 | 1 | -0.00491 | -3.6664 | -0.07411 |
| 34 | 6 | -3.28213 | -4.57021 | -0.37718 |
| 35 | 1 | -4.90369 | -3.13396 | -0.47012 |
| 36 | 1 | -1.41914 | -5.6602 | -0.17173 |
| 37 | 7 | -2.85704 | 6.427916 | -0.45405 |
| 38 | 6 | -2.08052 | 7.612092 | -0.26096 |
| 39 | 6 | -4.27141 | 6.628871 | -0.41295 |
| 40 | 6 | -3.3805 | 8.454984 | 0.821338 |
| 41 | 6 | -1.06988 | 7.98215 | -1.15617 |
| 42 | 6 | -4.82572 | 7.357419 | 0.651869 |
| 43 | 6 | -5.10887 | 6.169811 | -1.43649 |
| 44 | 6 | -1.64326 | 9.624088 | 1.031033 |
| 45 | 16 | -3.73379 | 8.01735 | 1.902231 |
| 46 | 6 | -0.31863 | 9.134736 | -0.93075 |
| 47 | 1 | -0.8715 | 7.351168 | -2.01689 |
| 48 | 6 | -6.20496 | 7.576475 | 0.714918 |
| 49 | 6 | -6.48684 | 6.366725 | -1.35866 |
| 50 | 1 | -4.67079 | 5.64682 | -2.28082 |
| 51 | 6 | -0.5985 | 9.951077 | 0.167881 |
| 52 | 1 | -1.89559 | 10.27409 | 1.863792 |
| 53 | 1 | 0.475417 | 9.401897 | -1.62207 |
| 54 | 1 | -6.61843 | 8.153852 | 1.536708 |
| 55 | 6 | -7.03652 | 7.061564 | -0.27849 |
| 56 | 1 | -7.12869 | 5.989744 | -2.14968 |
| 57 | 1 | -0.02081 | 10.85482 | 0.339475 |
| 58 | 1 | -8.10893 | 7.224536 | -0.22119 |
| 59 | 7 | -4.10631 | -5.71572 | -0.45166 |
| 60 | 6 | -5.53212 | -5.62363 | -0.41882 |
| 61 | 6 | -3.58884 | -7.03274 | -0.2512 |
| 62 | 6 | -6.22947 | -6.22029 | 0.643994 |
| 63 | 6 | -6.25252 | -5.00668 | -1.44845 |
| 64 | 6 | -4.0606 | -7.79301 | 0.831062 |
| 65 | 6 | -2.67005 | -7.60437 | -1.13935 |
| 66 | 6 | -7.62473 | -6.1532 | 0.698879 |
| 67 | 16 | -5.30224 | -7.08485 | 1.902539 |
| 68 | 6 | -7.6421 | -4.91807 | -1.37879 |
### Center Atomic Coordinates (Angstroms)

| Number | Number | X        | Y        | Z       |
|--------|--------|----------|----------|---------|
| 1      | 6      | -5.71219 | -4.58673 | 2.29106 |
| 70     | 6      | -3.57862 | -9.0872  | 1.047938|
| 71     | 6      | -2.17105 | -8.8852  | -0.90669|
| 72     | 1      | -2.3424  | -7.03019 | -2.00033|
| 73     | 6      | -8.32812 | -5.48269 | -0.30069|
| 74     | 1      | -8.15194 | -6.63144 | 1.519243|
| 75     | 1      | -8.18902 | -4.42062 | -2.17456|
| 76     | 1      | -3.96292 | -9.66916 | 1.880587|
| 77     | 6      | -2.61772 | -9.62347 | 0.192028|
| 78     | 1      | -1.4444  | -9.31113 | -1.59252|
| 79     | 1      | -9.41153 | -5.4233  | -0.24974|
| 80     | 1      | -2.23754 | -10.6255 | 0.369233|
| 81     | 7      | 6.991238 | -0.71912 | 0.497831|
| 82     | 6      | 7.8758   | 0.40082  | 0.423042|
| 83     | 6      | 7.632828 | -1.993   | 0.408219|
| 84     | 6      | 8.825666 | 0.451189 | -0.60995|
| 85     | 6      | 7.858689 | 1.416524 | 1.386283|
| 86     | 6      | 8.554204 | -2.22055 | -0.62682|
| 87     | 6      | 7.411495 | -2.99615 | 1.359261|
| 88     | 6      | 9.709687 | 1.530038 | -0.70412|
| 89     | 16     | 8.89686 | -0.89839 | -1.77824|
| 90     | 6      | 8.723401 | 2.504506 | 1.275869|
| 91     | 1      | 7.153395 | 1.35076  | 2.208802|
| 92     | 6      | 9.20348 | -3.45378 | -0.73552|
| 93     | 6      | 8.040098 | -4.23426 | 1.234246|
| 94     | 1      | 6.733535 | -2.79998 | 2.183986|
| 95     | 6      | 9.642622 | 2.566621 | 0.225664|
| 96     | 1      | 10.44878 | 1.548805 | -1.49978|
| 97     | 1      | 8.688285 | 3.295837 | 2.019076|
| 98     | 1      | 9.924436 | -3.61092 | -1.53252|
| 99     | 6      | 8.928774 | -4.46703 | 0.181744|
| 100    | 1      | 7.846243 | -5.01133 | 1.967982|
| 101    | 1      | 10.32398 | 3.408624 | 0.143791|
| 102    | 1      | 9.427113 | -5.4277  | 0.088524|

**Conformer E-1**

Total energy: $E(RB3LYP) = -3716.78099676$ a.u.
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 5 | 7 | 1.328953 | 0.32816 | -5E-06 |
| 6 | 7 | -0.3805 | -1.3155 | 0.000023 |
| 7 | 6 | 0.776 | 2.685338 | -4.2E-05 |
| 8 | 6 | -0.18961 | 3.704281 | -6.4E-05 |
| 9 | 6 | 2.135198 | 3.03364 | -4.2E-05 |
| 10 | 6 | 0.196555 | 5.041265 | -8.6E-05 |
| 11 | 1 | -1.23926 | 3.43432 | -5.8E-05 |
| 12 | 6 | 2.520832 | 4.371075 | -6.3E-05 |
| 13 | 1 | 2.879915 | 2.246306 | -2.6E-05 |
| 14 | 6 | 1.55916 | 5.383086 | -8.6E-05 |
| 15 | 1 | -0.5513 | 5.828842 | 0.0001 |
| 16 | 1 | 3.570738 | 4.646761 | -0.0006 |
| 17 | 6 | -2.71412 | -0.67072 | 0.00003 |
| 18 | 6 | -3.1137 | -2.01645 | 0.000339 |
| 19 | 6 | -3.69537 | 0.332208 | -0.00033 |
| 20 | 6 | -4.46464 | -2.35052 | 0.000334 |
| 21 | 1 | -2.35507 | -2.79047 | 0.00061 |
| 22 | 6 | -5.04644 | -0.00254 | -0.00036 |
| 23 | 1 | -3.38586 | 1.370816 | -0.00059 |
| 24 | 6 | -5.44037 | -1.3442 | -3.3E-05 |
| 25 | 1 | -4.77275 | -3.39197 | 0.000632 |
| 26 | 1 | -5.81016 | 0.768844 | -0.00064 |
| 27 | 6 | 1.937387 | -2.01518 | 0.000036 |
| 28 | 6 | 1.559539 | -3.36646 | -8E-06 |
| 29 | 6 | 3.302609 | -1.68832 | 0.000103 |
| 30 | 6 | 2.525042 | -4.36909 | 0.00013 |
| 31 | 1 | 0.505345 | -3.61782 | -6.6E-05 |
| 32 | 6 | 4.267437 | -2.69117 | 0.000126 |
| 33 | 1 | 3.593582 | -0.6443 | 0.000135 |
| 34 | 6 | 3.883897 | -4.03937 | 0.000081 |
| 35 | 1 | 2.238906 | -5.4162 | -2.2E-05 |
| 36 | 1 | 5.323399 | -2.43719 | 0.00018 |
| 37 | 7 | -6.84339 | -1.65417 | -5.1E-05 |
| 38 | 6 | -7.46543 | -1.97204 | -1.23829 |
| 39 | 6 | -7.46565 | -1.97106 | 1.238325 |
| 40 | 6 | -8.86879 | -1.93417 | -1.35433 |
| 41 | 6 | -6.71754 | -2.31688 | -2.37476 |
| 42 | 6 | -8.86904 | -1.93313 | 1.354071 |
| 43 | 6 | -6.71795 | -2.31499 | 2.375204 |
| 44 | 6 | -9.49316 | -2.27448 | -2.555 |
| 45 | 16 | -9.85619 | -1.33154 | -0.00044 |
| 46 | 6 | -7.34797 | -2.61431 | -3.58353 |
| 47 | 1 | -5.63603 | -2.34231 | -2.32035 |
| 48 | 6 | -9.49361 | -2.27255 | 2.554893 |
| 49 | 6 | -7.3486 | -2.61151 | 3.584079 |
| 50 | 1 | -5.63643 | -2.34043 | 2.321002 |
| 51 | 6 | -8.73743 | -2.60475 | -3.68009 |
| 52 | 1 | -10.5783 | -2.25675 | -2.60611 |
|   |   |       |       |       |       |
|---|---|-------|-------|-------|-------|
| 53 | 1 | -6.7395 | -2.86575 | -4.44779 |
| 54 | 1 | -10.5787 | -2.25482 | 2.605782 |
| 55 | 6 | -8.73809 | -2.60193 | 3.680378 |
| 56 | 1 | -6.74029 | -2.86224 | 4.448658 |
| 57 | 1 | -9.23141 | -2.84806 | -4.616 |
| 58 | 1 | -9.23223 | -2.84456 | 4.616372 |
| 59 | 7 | 4.853894 | -5.0994 | 0.000106 |
| 60 | 6 | 5.440246 | -5.47906 | -1.23818 |
| 61 | 6 | 5.440147 | -5.47908 | 1.238426 |
| 62 | 6 | 6.109745 | -6.71302 | -1.35403 |
| 63 | 6 | 5.36433 | -4.65926 | -2.37483 |
| 64 | 6 | 6.109637 | -6.71305 | 1.354311 |
| 65 | 6 | 5.364141 | -4.6593 | 2.375087 |
| 66 | 6 | 6.716666 | -7.08355 | -2.55472 |
| 67 | 16 | 6.082382 | -7.86913 | 0.000126 |
| 68 | 6 | 5.937178 | -5.05648 | -3.58358 |
| 69 | 1 | 4.845106 | -3.71019 | -2.32058 |
| 70 | 6 | 6.716462 | -7.0836 | 2.555035 |
| 71 | 6 | 5.936893 | -5.05655 | 3.58388 |
| 72 | 1 | 4.844923 | -3.71023 | 2.320815 |
| 73 | 6 | 6.624247 | -6.26424 | -3.67998 |
| 74 | 1 | 7.244352 | -8.03187 | -2.60567 |
| 75 | 1 | 5.850232 | -4.40406 | -4.44798 |
| 76 | 1 | 7.244143 | -8.03193 | 2.606017 |
| 77 | 6 | 6.623953 | -6.26431 | 3.680304 |
| 78 | 1 | 5.849879 | -4.40415 | 4.448285 |
| 79 | 1 | 7.081989 | -6.57034 | -4.61588 |
| 80 | 1 | 7.08162 | -6.57043 | 4.616234 |
| 81 | 7 | 1.989073 | 6.753085 | -0.00011 |
| 82 | 6 | 2.025278 | 7.450585 | -1.23842 |
| 83 | 6 | 2.025226 | 7.45064 | 1.238175 |
| 84 | 6 | 2.759988 | 8.646868 | -1.35432 |
| 85 | 6 | 1.35293 | 6.97532 | -2.37503 |
| 86 | 6 | 2.759929 | 8.646929 | 1.354051 |
| 87 | 6 | 1.352834 | 6.975422 | 2.374777 |
| 88 | 6 | 2.777916 | 9.357639 | -2.55505 |
| 89 | 16 | 3.775193 | 9.200584 | -0.00012 |
| 90 | 6 | 1.411023 | 7.669906 | -3.58383 |
| 91 | 1 | 0.789954 | 6.05153 | -2.32068 |
| 92 | 6 | 2.777804 | 9.357753 | 2.55475 |
| 93 | 6 | 1.410875 | 7.670062 | 3.583554 |
| 94 | 1 | 0.789865 | 6.051626 | 2.320448 |
| 95 | 6 | 2.114273 | 8.868307 | -3.68029 |
| 96 | 1 | 3.335975 | 10.28841 | -2.60606 |
| 97 | 1 | 0.889223 | 7.268705 | -4.44822 |
| 98 | 1 | 3.33586 | 10.28853 | 2.605746 |
| 99 | 6 | 2.114116 | 8.86847 | 3.679986 |
| 100 | 1 | 0.889042 | 7.268897 | 4.447935 |
Conformer E-2
Total energy: E(RB3LYP) = -3716.78134568 a.u.

| Center Number | Atomic Number | X     | Y     | Z      |
|---------------|---------------|-------|-------|--------|
| 1             | 6             | 0.299563 | 1.252114 | -9.3E-05 |
| 2             | 7             | 1.296958 | 0.354727 | -0.00013 |
| 3             | 6             | 0.922452 | -0.93381 | -0.00022 |
| 4             | 6             | -1.28204 | -0.38029 | -0.00026 |
| 5             | 7             | -1.00319 | 0.932219 | -0.00013 |
| 6             | 7             | -0.35329 | -1.3484  | -0.00027 |
| 7             | 6             | 0.66057  | 2.69087  | 0.000049 |
| 8             | 6             | 2.007628 | 3.085846 | -0.00001 |
| 9             | 6             | -0.33887 | 3.67565  | 0.000229 |
| 10            | 6             | 2.346434 | 4.435607 | 0.000116 |
| 11            | 1             | 2.778961 | 2.324467 | -0.00019 |
| 12            | 6             | 0.000558 | 5.025593 | 0.000377 |
| 13            | 1             | -1.37853 | 3.369698 | 0.000269 |
| 14            | 6             | 1.343532 | 5.414844 | 0.00035 |
| 15            | 1             | 3.388908 | 4.740304 | 0.000001 |
| 16            | 1             | -0.76818 | 5.791987 | 0.000536 |
| 17            | 6             | 1.987315 | -1.96625 | -0.00027 |
| 18            | 6             | 1.656583 | -3.32984 | -0.00043 |
| 19            | 6             | 3.340365 | -1.59223 | -0.00014 |
| 20            | 6             | 2.656355 | -4.29834 | -0.00049 |
| 21            | 1             | 0.611778 | -3.61772 | -0.00053 |
| 22            | 6             | 4.339446 | -2.56094 | -0.00018 |
| 23            | 1             | 3.594886 | -0.53872 | 0.000015 |
| 24            | 6             | 4.002928 | -3.92167 | -0.00038 |
| 25            | 1             | 2.406548 | -5.3547  | -0.00064 |
| 26            | 1             | 5.386001 | -2.27056 | -0.00004 |
| 27            | 6             | -2.70827 | 0.786822 | -0.00019 |
| 28            | 6             | -3.06142 | -2.14479 | -0.00018 |
| 29            | 6             | -3.72362 | 0.182602 | -0.00014 |
| 30            | 6             | -4.4003  | -2.52546 | -0.00014 |
| 31            | 1             | -2.27689 | -2.89246 | -0.00022 |
| 32            | 6             | -5.06197 | -0.19864 | -0.00009 |
| 33            | 1             | -3.44986 | 1.231268 | -0.00013 |
| 34            | 6             | -5.4087  | -1.5568  | -9.9E-05 |
| 35            | 1             | -4.67975 | -3.57436 | -0.00014 |
| 36            | 1             | -5.84682 | 0.552066 | -2.5E-05 |
| 37 | 7 | 5.009313 | -4.94723 | -0.0004 |
| 38 | 6 | 5.608467 | -5.30648 | -1.23858 |
| 39 | 6 | 5.607509 | -5.30727 | 1.23802 |
| 40 | 6 | 6.320068 | -6.51666 | -1.35453 |
| 41 | 6 | 5.504553 | -4.48962 | -2.37513 |
| 42 | 6 | 6.318973 | -6.51755 | 1.353801 |
| 43 | 6 | 5.502796 | -4.49104 | 2.374947 |
| 44 | 6 | 6.939513 | -6.86587 | -2.5552 |
| 45 | 16 | 6.332216 | -7.67341 | -0.00073 |
| 46 | 6 | 6.090826 | -4.86672 | -3.58389 |
| 47 | 1 | 4.952701 | -3.55915 | -2.32077 |
| 48 | 6 | 6.93745 | -6.8675 | 2.554753 |
| 49 | 6 | 6.088098 | -4.86889 | 3.583945 |
| 50 | 1 | 4.951093 | -3.56047 | 2.320665 |
| 51 | 6 | 6.819083 | -6.05009 | -3.68037 |
| 52 | 1 | 7.499427 | -7.79553 | -2.60624 |
| 53 | 1 | 5.981311 | -4.21773 | -4.4483 |
| 54 | 1 | 7.497282 | -7.79722 | 2.605689 |
| 55 | 6 | 6.816179 | -6.05237 | 3.68031 |
| 56 | 1 | 5.977976 | -4.22038 | 4.448651 |
| 57 | 1 | 7.287023 | -6.34024 | -4.6163 |
| 58 | 1 | 7.283357 | -6.34311 | 4.616444 |
| 59 | 7 | -6.78037 | -1.98469 | -2.3E-05 |
| 60 | 6 | -7.47764 | -2.01868 | 1.238455 |
| 61 | 6 | -7.47816 | -2.01777 | -1.23822 |
| 62 | 6 | -8.67731 | -2.74789 | 1.354312 |
| 63 | 6 | -6.9988 | -1.3495 | 2.375451 |
| 64 | 6 | -8.67791 | -2.74685 | -1.35406 |
| 65 | 6 | -6.99978 | -1.34788 | -2.37498 |
| 66 | 6 | -9.3877 | -2.76336 | 2.555299 |
| 67 | 16 | -9.23623 | -3.75986 | -0.00013 |
| 68 | 6 | -7.69318 | -1.40528 | 3.584483 |
| 69 | 1 | -6.0723 | -0.79101 | 2.321296 |
| 70 | 6 | -9.38885 | -2.76144 | -2.55473 |
| 71 | 6 | -7.6947 | -1.40277 | -3.58374 |
| 72 | 1 | -6.07318 | -0.78952 | -2.32089 |
| 73 | 6 | -8.89486 | -2.1029 | 3.680873 |
| 74 | 1 | -10.321 | -3.31718 | 2.606226 |
| 75 | 1 | -7.28908 | -0.88618 | 4.449149 |
| 76 | 1 | -10.322 | -3.31517 | -2.60562 |
| 77 | 6 | -8.89649 | -2.10021 | -3.68007 |
| 78 | 1 | -7.29094 | -0.88313 | -4.44824 |
| 79 | 1 | -9.44401 | -2.13772 | 4.617012 |
| 80 | 1 | -9.44607 | -2.13434 | -4.61598 |
| 81 | 7 | 1.658629 | 6.816719 | 0.000415 |
| 82 | 6 | 1.97939 | 7.43736 | 1.238601 |
| 83 | 6 | 1.97769 | 7.437619 | -1.23807 |
| 84 | 6 | 1.948476 | 8.840922 | 1.354561 |
| Conformers | 1 (Ha)     | 2 (Ha)     | ∆E* (eV) | ∆E(E-A)** (eV) |
|------------|------------|------------|----------|----------------|
| Equatorial | -3716.864284 | -3716.864231 | -0.0014  | 0.051          |
| Axial      | -3716.866069 | -3716.866167 | -0.0027  |                |

* Energy difference between conformers with similar structure.  ** Energy difference between equatorial-1 and axial conformer-1.

Table S3 Energies (in eV) of the frontier molecular orbitals for the E-1 and A-1 conformers. This was calculated at the B3LYP/6-31G* level of theory.

| Conformers | HOMO-2 | HOMO-1 | HOMO | LUMO | LUMO+1 |
|------------|--------|--------|------|------|--------|
| E-1        | -5.07  | -5.07  | -5.07| -2.33| -2.33  |
| A-1        | -5.20  | -5.20  | -5.18| -1.25| 1.25   |
Table S4: Configuration interaction descriptions of S1 and T1 for the E-1 and A-1 conformers. This was calculated at the B3LYP/6-31G* level of theory.

| Conformer | State | Initial → Final          | Contribution% |
|-----------|-------|--------------------------|---------------|
| **E-1**   |       |                          |               |
|           | T1    | HOMO → LUMO              | 78.98         |
|           |       | HOMO → LUMO+1            | 13.26         |
|           |       | HOMO-1 → LUMO+1          | 4.49          |
|           |       | HOMO → LUMO              | 70.44         |
|           | S1    | HOMO-1 → LUMO+1          | 12.34         |
|           |       | HOMO → LUMO+1            | 12.18         |
| **A-1**   |       |                          |               |
|           | T1    | HOMO-1 → LUMO            | 30.15         |
|           |       | HOMO-2 → LUMO+1          | 30.09         |
|           |       | HOMO-2 → LUMO            | 8.55          |
|           |       | HOMO-1 → LUMO+1          | 8.54          |
|           | S1    | HOMO-2 → LUMO            | 37.67         |
|           |       | HOMO-1 → LUMO+1          | 37.63         |
|           |       | HOMO-1 → LUMO            | 10.71         |
|           |       | HOMO-2 → LUMO+1          | 10.64         |