# Cross-Plane Magnetic Coupling in Carbon-Based Diradicals with One-Electron σ-Bond Regulated by Conjugative Substituent Engineering

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## Electronic Supplementary Information

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**Section S1**. The isosurface diagrams of orbital distributions of SOMO1 and SOMO2 in systems with different types and positions of substituents.

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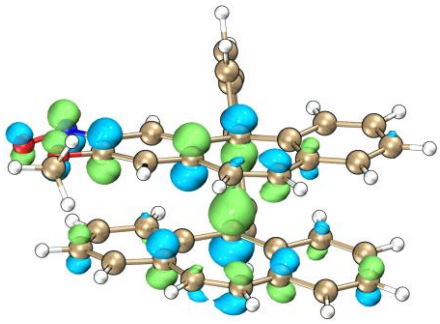
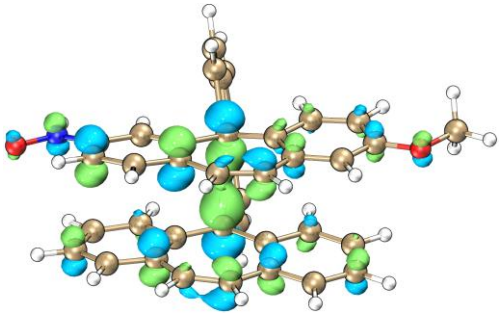
|  |  |
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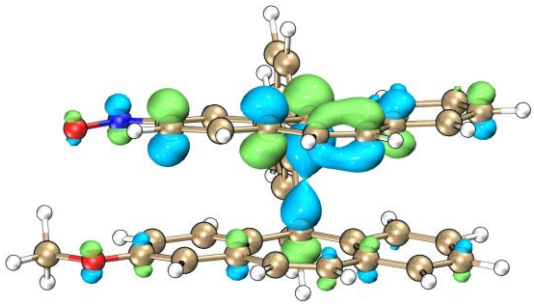
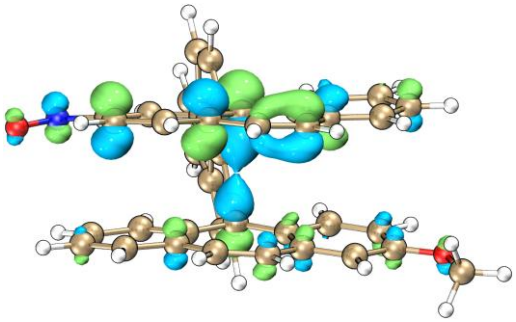
|  |  |
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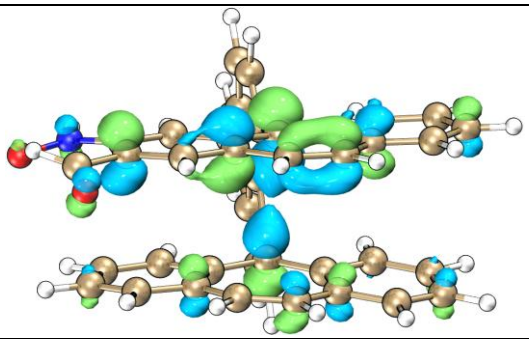
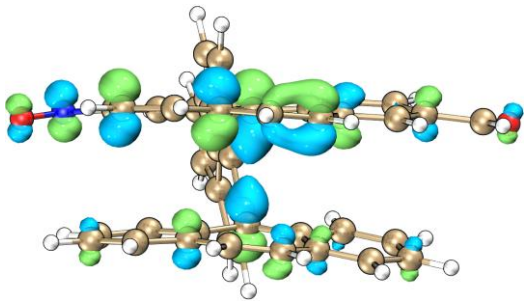
|  |  |
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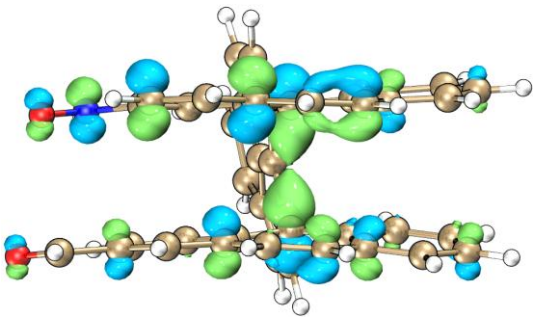
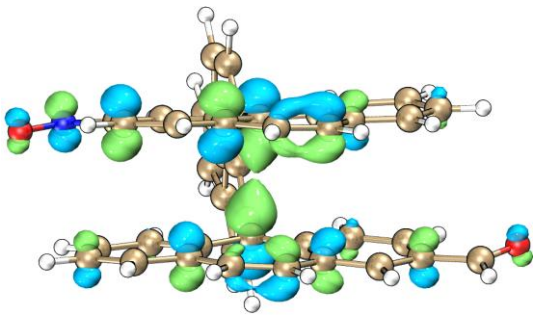
|  |  |
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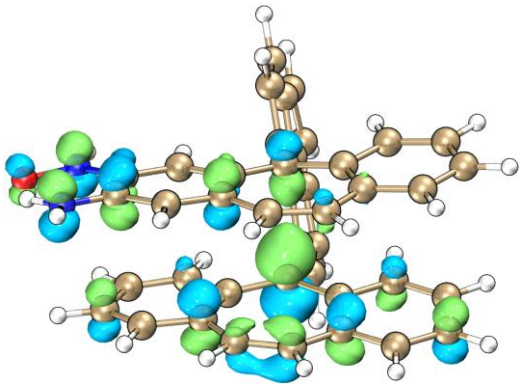
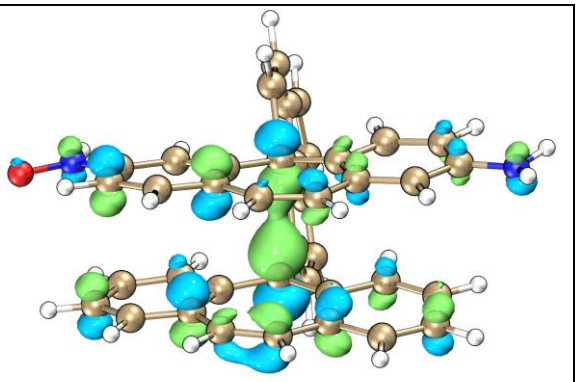
|  |  |
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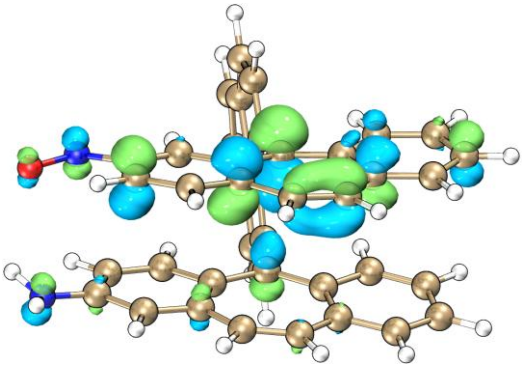
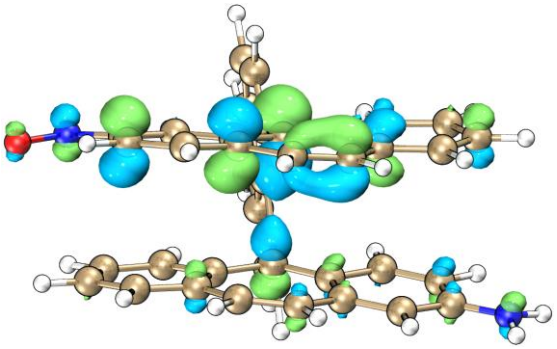
|  |  |
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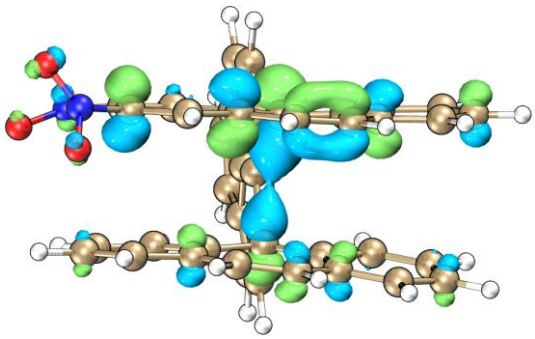
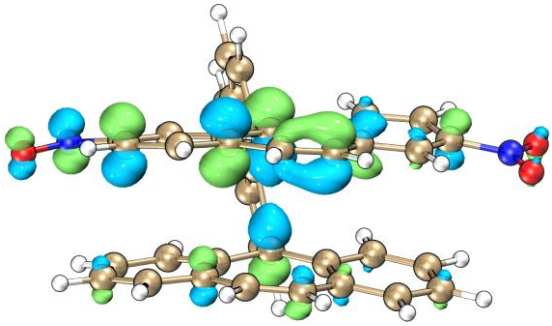
|  |  |
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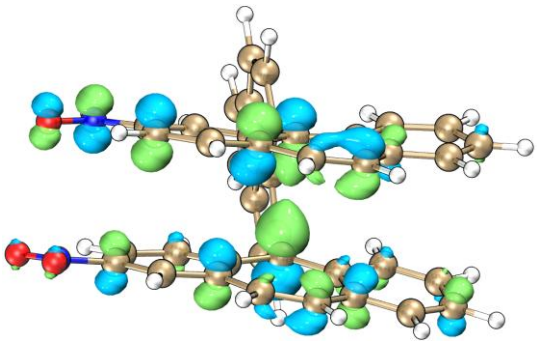
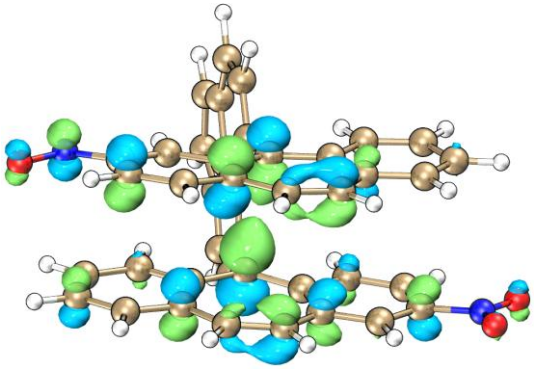
|  |  |
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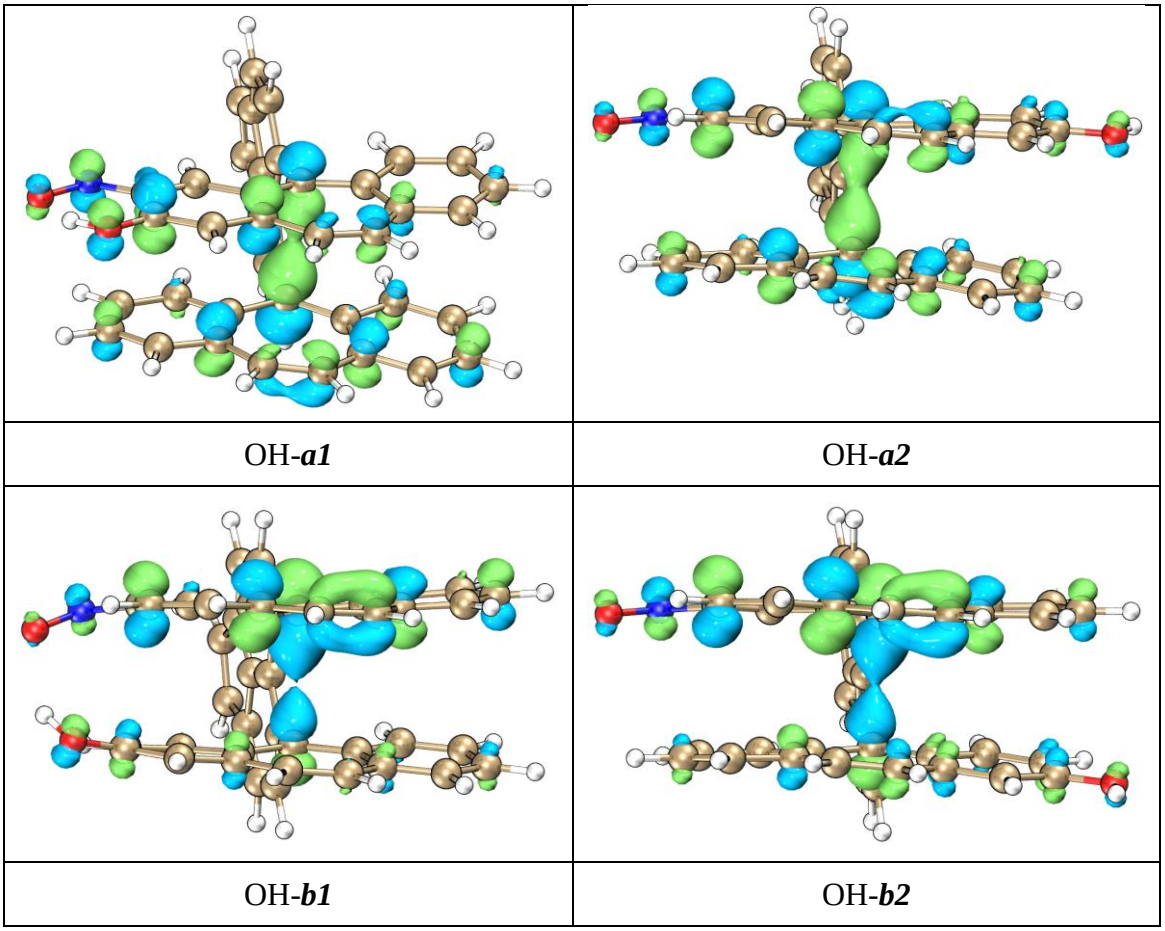


**Figure S1.** The isosurface diagram of orbital distribution of SOMO1 in systems with different types and positions of substituents.

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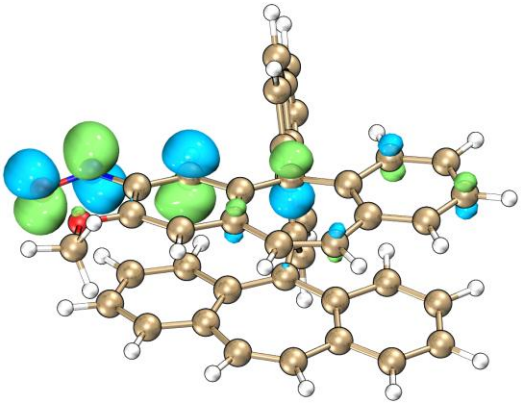
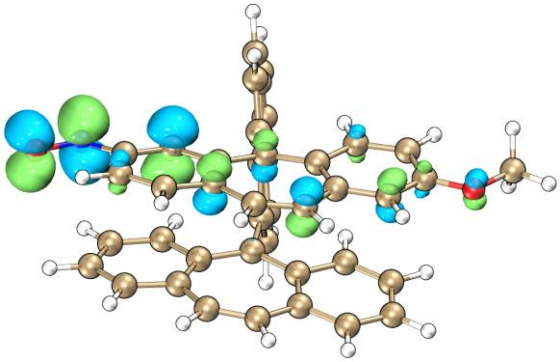
|  |  |
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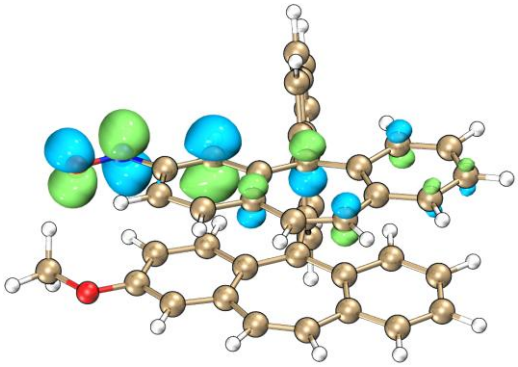
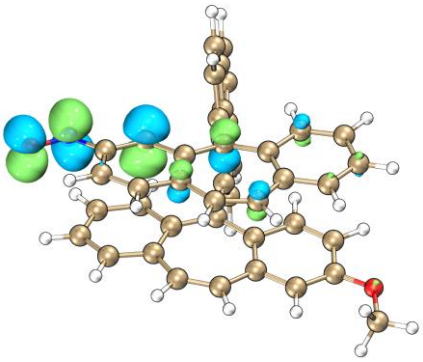
|  |  |
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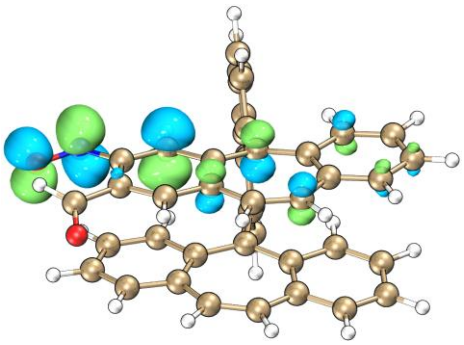
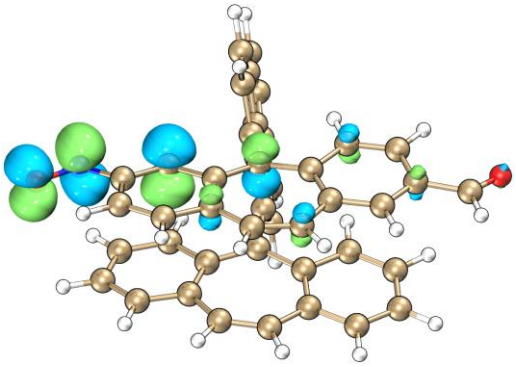
|  |  |
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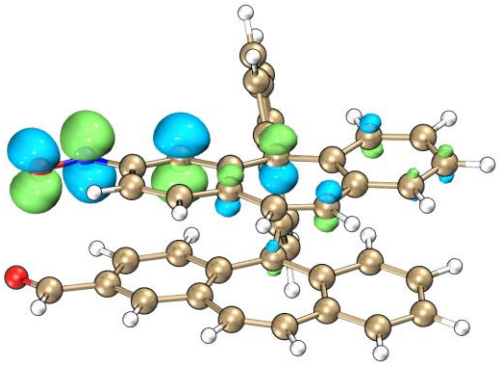
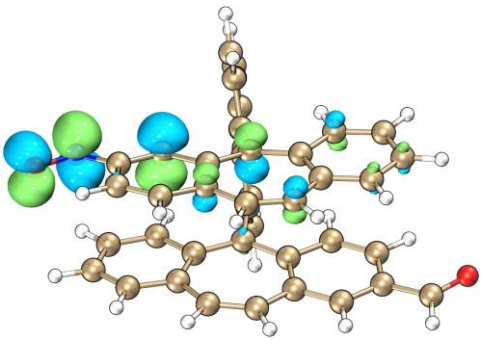
|  |  |
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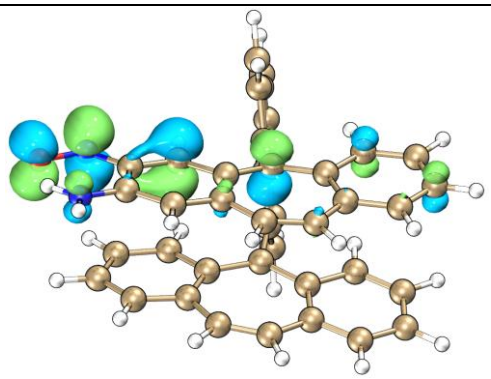
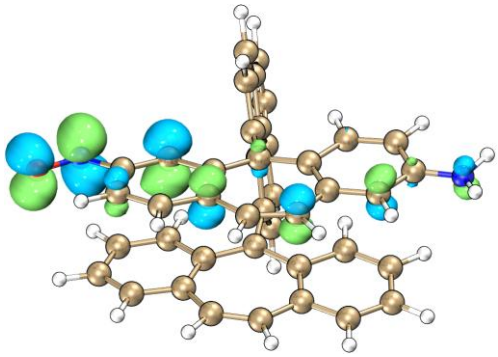
|  |  |
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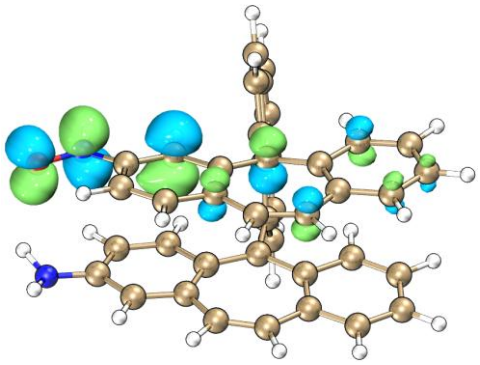
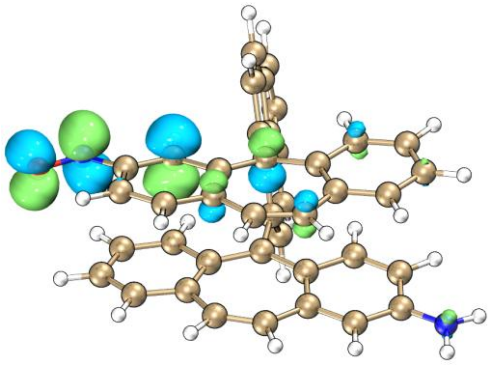
|  |  |
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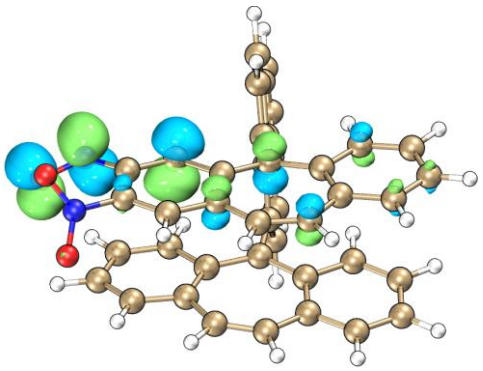
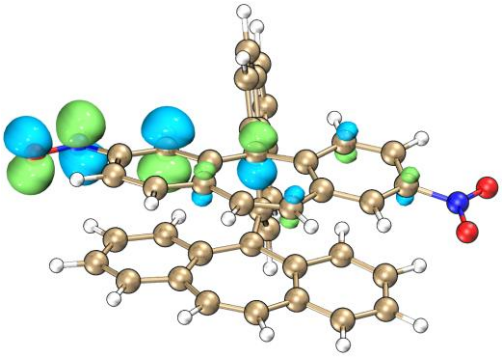
|  |  |
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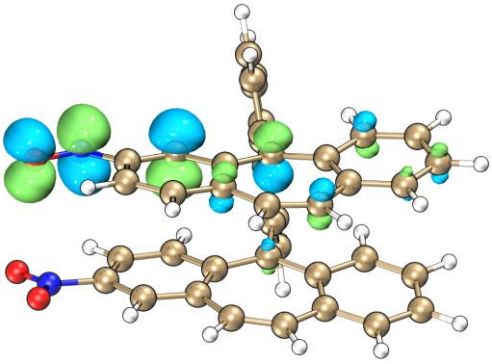
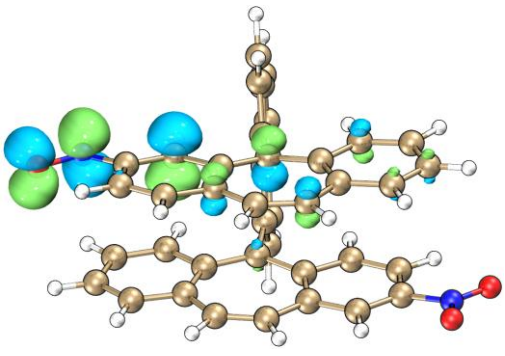
|  |  |
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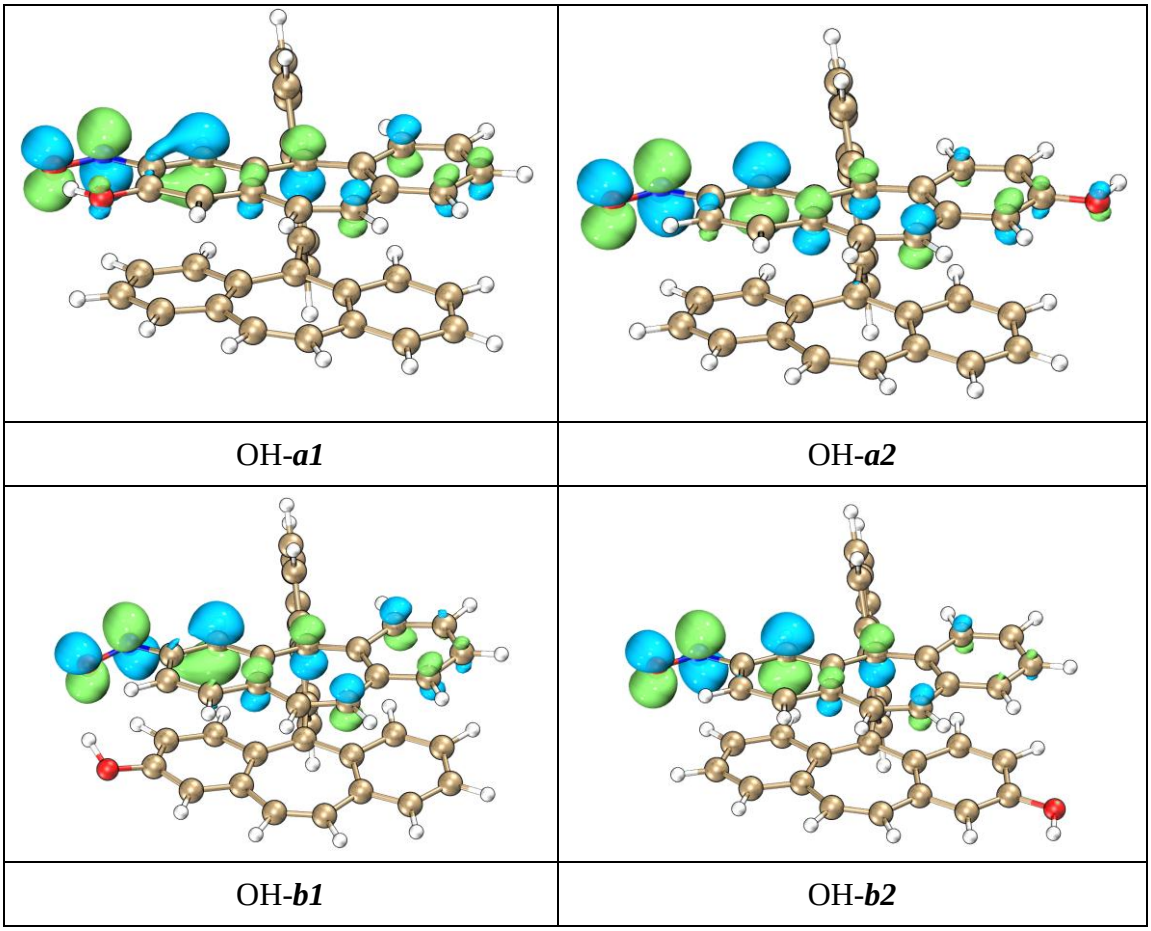


**Figure S2.** The isosurface diagram of orbital distribution of SOMO2 in systems with different types and positions of substituents.

**Section S2**. The isosurface diagrams of spin density distributions in systems with different types and positions of substituents

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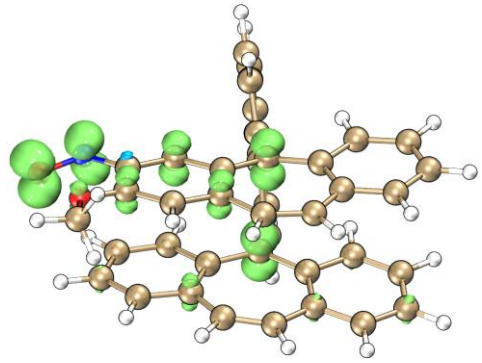
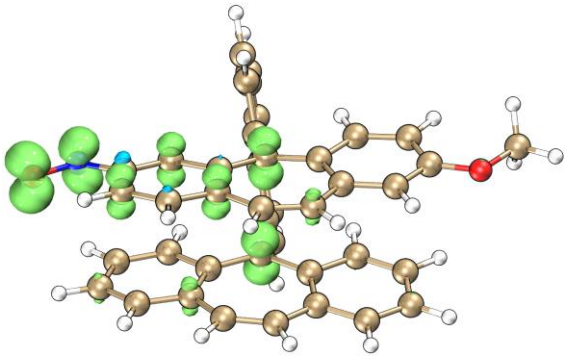
|  |  |
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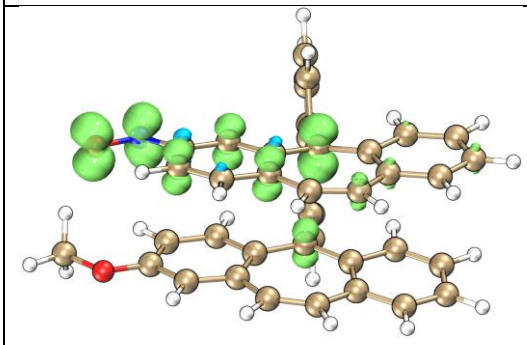
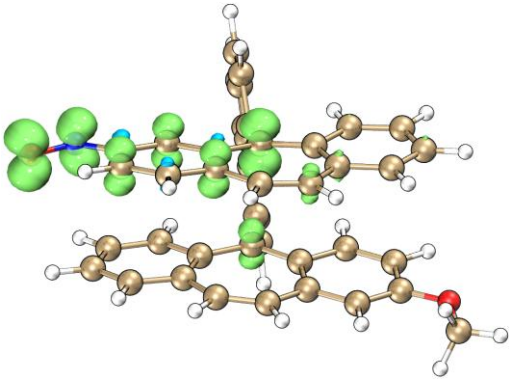
|  |  |
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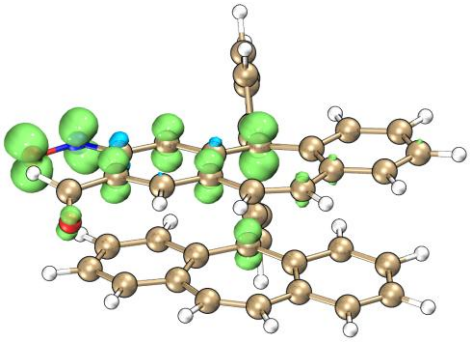
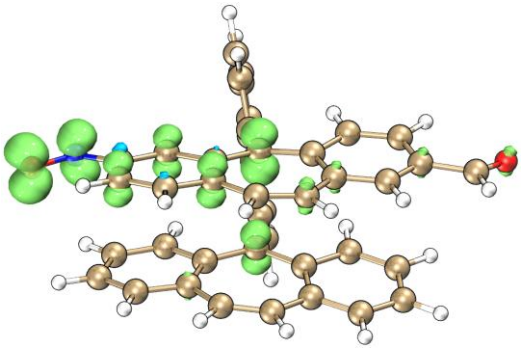
|  |  |
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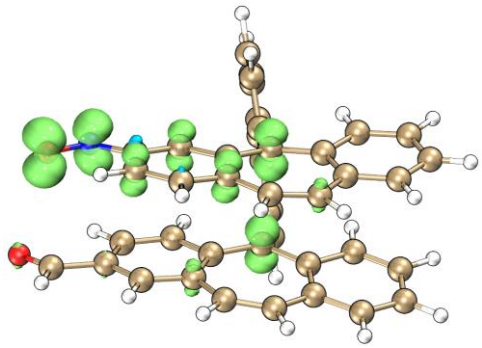
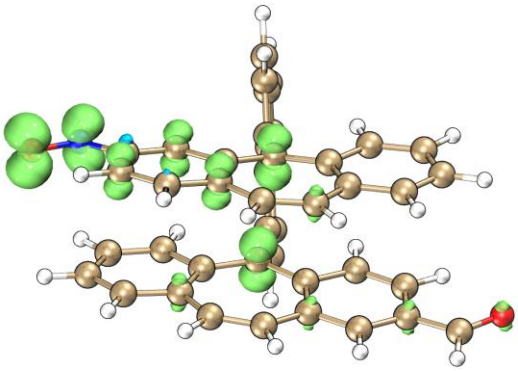
|  |  |
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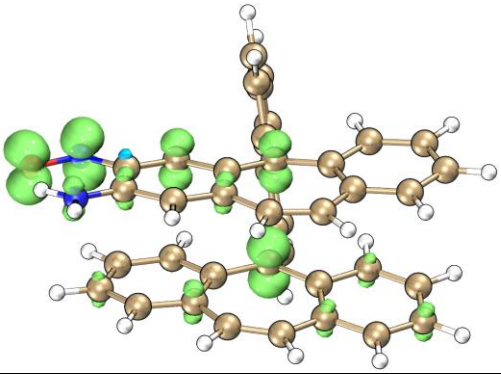
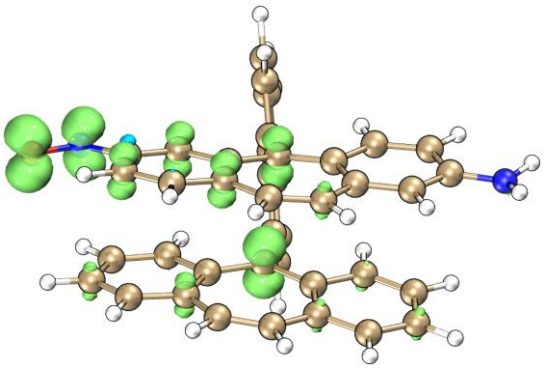
|  |  |
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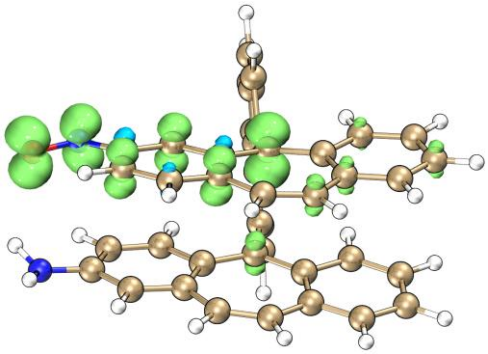
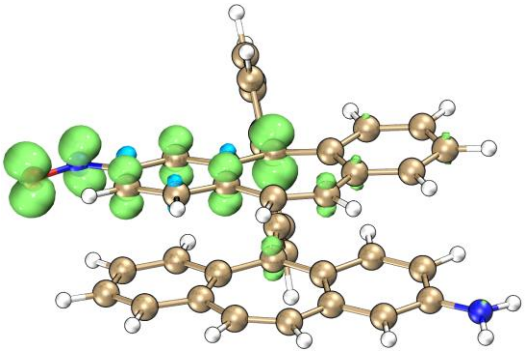
|  |  |
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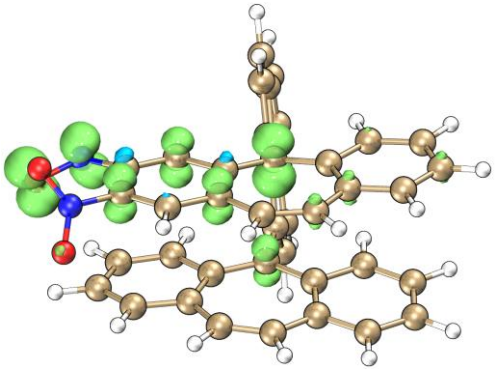
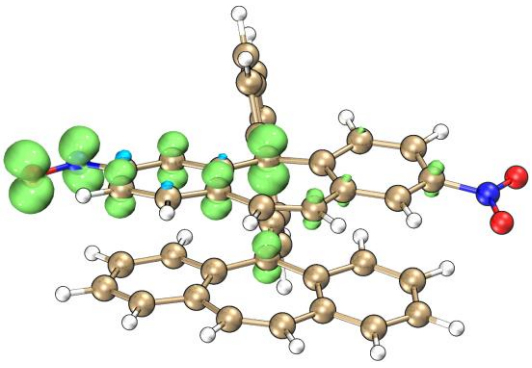
|  |  |
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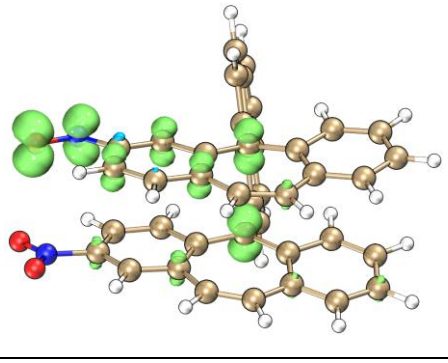
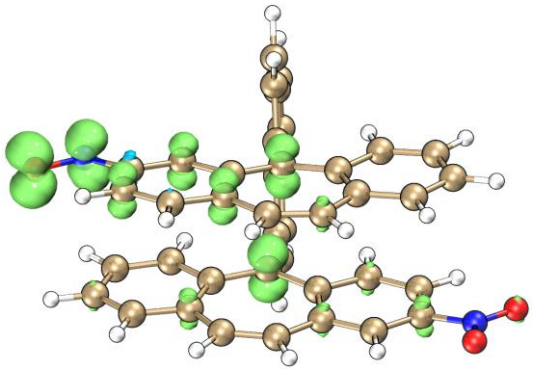
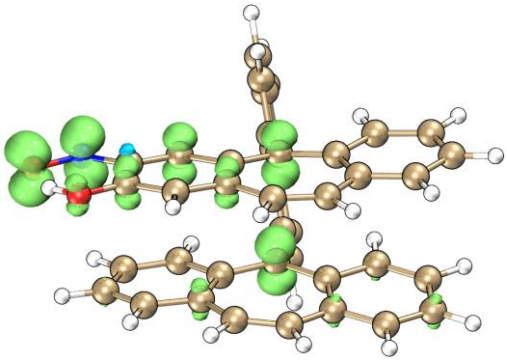
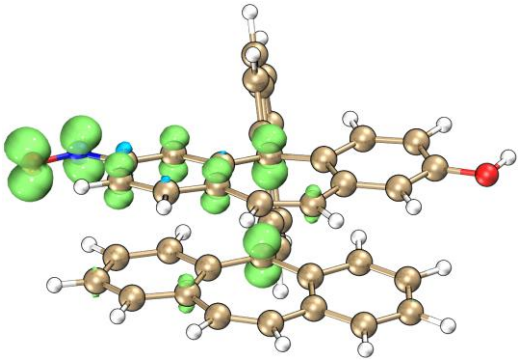
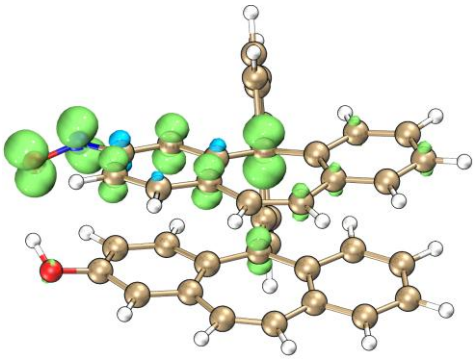
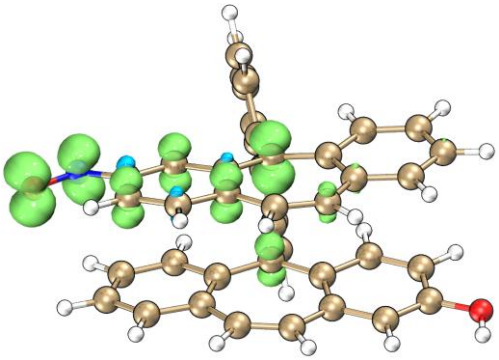
|  |  |
| $NO_2$-***b1*** | $NO_2$-***b2*** |
|  |  |
| OH-***a1*** | OH-***a2*** |
|  |  |
| OH-***b1*** | OH-***b2*** |

**Figure S3.** The isosurface diagram of spin density distribution in systems with different types and positions of substituents.

**Section S3**. Annotation for distinguishing atoms that contribute differently to the orbital composition of SOMO (Figure S4) and the contributions of atoms to SOMO1 (Table S2) and SOMO2 (Table S3), respectively

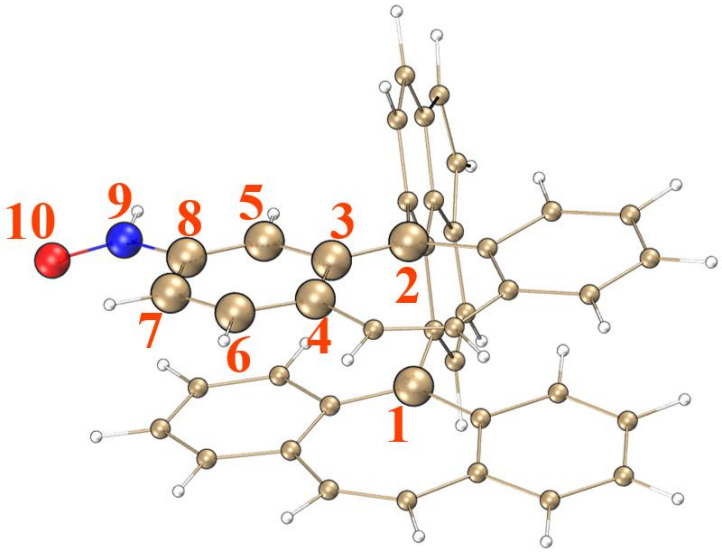



**Figure S4.** Annotate to distinguish atoms that contribute differently to the orbital composition of SOMO.

**Section S4**. Parallel verification of different calculation methods

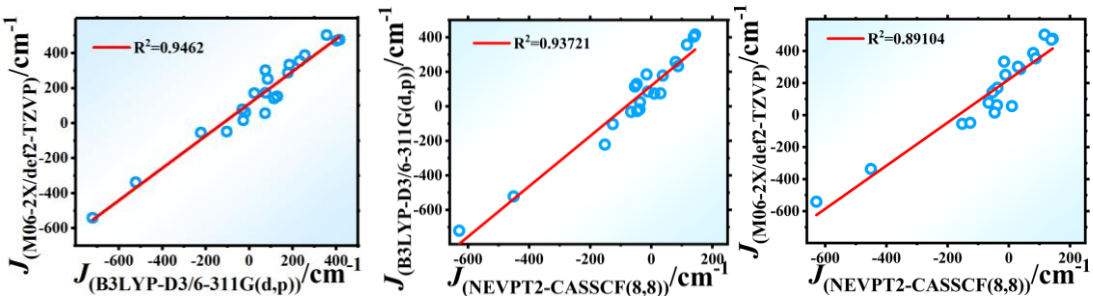



**Figure S5.** Parallel verification of different calculation methods.

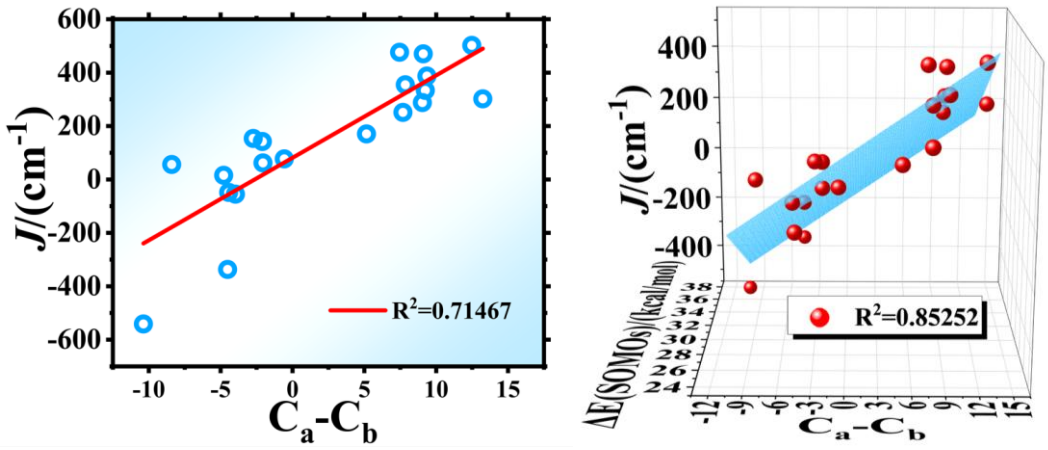



**Figure S6.** The linear fitting between the difference in contributions of $C_a$ and $C_b$ to SOMO1 and the magnetic coupling constant $J$， and the planar fitting among the difference in contributions of $C_a$ and $C_b$ to SOMO1, the SOMO gap, and the magnetic coupling constant $J$ (M06-2x/def2-TZVP).

**Section S5**. Becke-based population analysis, the spin population at $C_a$ and $C_b$

**Table S1.** Becke-based population analysis, the spin population at $C_a$ and $C_b$ (B3LYP-D3/6-311G(d,p)).

| | **Substituent position** | **$C_a$** | **$C_b$** |
|---|---|---|---|
| origin | - | 0.216 | 0.170 |
| $-OCH_3$ | ***a1*** | 0.184 | 0.215 |
| | ***a2*** | 0.178 | 0.210 |
| | ***b1*** | 0.265 | 0.126 |
| | ***b2*** | 0.265 | 0.118 |
| -CHO | ***a1*** | 0.244 | 0.129 |
| | ***a2*** | 0.228 | 0.148 |
| | ***b1*** | 0.189 | 0.187 |
| | ***b2*** | 0.179 | 0.197 |
| $-NH_2$ | ***a1*** | 0.155 | 0.258 |
| | ***a2*** | 0.142 | 0.243 |
| | ***b1*** | 0.303 | 0.090 |
| | ***b2*** | 0.290 | 0.088 |
| $-NO_2$ | ***a1*** | 0.262 | 0.121 |
| | ***a2*** | 0.245 | 0.132 |
| | ***b1*** | 0.169 | 0.213 |
| | ***b2*** | 0.161 | 0.216 |
| -OH | ***a1*** | 0.189 | 0.218 |
| | ***a2*** | 0.183 | 0.204 |
| | ***b1*** | 0.286 | 0.113 |
| | ***b2*** | 0.255 | 0.129 |

**Section S6**. According to the annotation in Figure S4, the contribution of atoms to SOMO1 and SOMO2.

**Table S2.** The contribution of atoms to SOMO1 (B3LYP-D3/6-311G(d,p)).

| | **Substituent** | **Contribution of atoms (%)** | | | | |
|---|---|---|---|---|---|---|
| | **position** | **1($C_b$)** | **2($C_a$)** | **3** | **4** | **5** |
| -$OCH_3$ | ***a1*** | 9.816 | 5.650 | 2.310 | 6.095 | 0.502 |
| | ***a2*** | 9.746 | 7.613 | 1.879 | 5.723 | 0.669 |
| | ***b1*** | 5.813 | 11.026 | 2.613 | 7.763 | 1.089 |
| | ***b2*** | 5.656 | 10.890 | 2.646 | 8.092 | 1.016 |
| -CHO | ***a1*** | 6.148 | 10.123 | 2.324 | 6.851 | 1.237 |
| | ***a2*** | 6.454 | 8.428 | 2.322 | 7.908 | 0.506 |
| | ***b1*** | 8.154 | 6.879 | 1.977 | 6.950 | 0.402 |
| | ***b2*** | 8.852 | 6.754 | 1.955 | 6.662 | 0.441 |
| -$NH_2$ | ***a1*** | 12.199 | 4.048 | 2.508 | 4.126 | 0.623 |
| | ***a2*** | 11.544 | 6.304 | 1.559 | 4.532 | 0.597 |
| | ***b1*** | 3.894 | 12.828 | 2.816 | 8.034 | 1.358 |
| | ***b2*** | 4.568 | 12.112 | 2.844 | 8.437 | 1.265 |
| -$NO_2$ | ***a1*** | 5.958 | 11.169 | 2.508 | 6.751 | 1.503 |
| | ***a2*** | 5.650 | 8.928 | 2.428 | 8.401 | 0.520 |
| | ***b1*** | 9.309 | 5.550 | 1.727 | 6.382 | 0.313 |
| | ***b2*** | 9.737 | 5.870 | 1.796 | 6.306 | 0.380 |
| -OH | ***a1*** | 10.521 | 6.391 | 2.588 | 5.085 | 0.835 |
| | ***a2*** | 9.464 | 7.800 | 1.936 | 5.942 | 0.672 |
| | ***b1*** | 5.708 | 12.043 | 2.671 | 6.974 | 1.520 |
| | ***b2*** | 6.147 | 10.322 | 2.558 | 7.943 | 0.918 |

| | Substituent position | Contribution of atoms (%) | | | | |
|---|---|---|---|---|---|---|
| | | **6** | **7** | **8** | **9** | **10** |
| -$OCH_3$ | ***a1*** | 1.369 | 5.312 | 2.382 | 4.338 | 2.919 |
| | ***a2*** | 1.650 | 5.094 | 1.352 | 2.037 | 1.097 |
| | ***b1*** | 2.402 | 6.598 | 1.874 | 2.158 | 1.111 |
| | ***b2*** | 2.307 | 7.033 | 1.808 | 2.344 | 1.323 |
| -CHO | ***a1*** | 2.845 | 6.271 | 1.558 | 1.447 | 0.793 |
| | ***a2*** | 2.245 | 6.575 | 1.899 | 3.653 | 2.313 |
| | ***b1*** | 1.970 | 5.821 | 1.662 | 3.568 | 2.296 |
| | ***b2*** | 1.948 | 5.602 | 1.678 | 3.115 | 1.843 |
| -$NH_2$ | ***a1*** | 1.167 | 4.577 | 2.948 | 3.907 | 2.294 |
| | ***a2*** | 1.363 | 4.109 | 1.122 | 1.622 | 0.807 |
| | ***b1*** | 2.558 | 6.764 | 1.798 | 2.043 | 1.292 |
| | ***b2*** | 2.384 | 7.402 | 1.835 | 2.091 | 1.163 |
| -$NO_2$ | ***a1*** | 2.521 | 6.080 | 1.628 | 1.424 | 0.802 |
| | ***a2*** | 2.308 | 6.984 | 1.947 | 3.896 | 2.563 |
| | ***b1*** | 1.757 | 5.424 | 1.617 | 4.156 | 3.018 |
| | ***b2*** | 1.854 | 5.289 | 1.641 | 3.089 | 1.815 |
| -OH | ***a1*** | 1.163 | 5.167 | 2.783 | 3.099 | 1.575 |
| | ***a2*** | 1.717 | 5.258 | 1.403 | 2.131 | 1.158 |
| | ***b1*** | 2.261 | 5.748 | 1.757 | 1.585 | 0.829 |
| | ***b2*** | 2.264 | 6.878 | 1.793 | 2.470 | 1.413 |

**Table S3.** The contribution of atoms to SOMO2 (B3LYP-D3/6-311G(d,p)).

| | Substituent | Contribution of atoms (%) | | | | |
|---|---|---|---|---|---|---|
| | position | 1($C_b$) | 2($C_a$) | 3 | 4 | 5 |
| -$OCH_3$ | ***a1*** | 1.358 | 6.012 | 2.280 | 1.980 | 12.072 |
| | ***a2*** | 1.167 | 2.740 | 1.949 | 4.324 | 10.962 |
| | ***b1*** | 0.800 | 5.006 | 2.326 | 3.307 | 13.281 |
| | ***b2*** | 0.890 | 4.879 | 2.327 | 3.009 | 13.173 |
| -CHO | ***a1*** | 0.873 | 4.580 | 2.319 | 3.436 | 13.024 |
| | ***a2*** | 1.269 | 5.408 | 2.372 | 2.565 | 12.805 |
| | ***b1*** | 1.616 | 4.917 | 2.266 | 2.683 | 12.481 |
| | ***b2*** | 1.411 | 4.633 | 2.238 | 2.942 | 12.500 |
| -$NH_2$ | ***a1*** | 0.995 | 6.880 | 2.726 | 1.803 | 11.309 |
| | ***a2*** | 1.052 | 1.766 | 1.837 | 5.232 | 9.971 |
| | ***b1*** | 0.865 | 5.181 | 2.349 | 3.260 | 13.544 |
| | ***b2*** | 0.649 | 4.852 | 2.337 | 3.047 | 13.352 |
| -$NO_2$ | ***a1*** | 0.630 | 4.242 | 2.151 | 3.215 | 11.967 |
| | ***a2*** | 1.210 | 5.803 | 2.455 | 2.375 | 13.000 |
| | ***b1*** | 1.621 | 5.240 | 2.302 | 2.581 | 12.433 |
| | ***b2*** | 1.465 | 4.580 | 2.231 | 2.918 | 12.420 |
| -OH | ***a1*** | 0.523 | 5.899 | 2.571 | 2.652 | 11.658 |
| | ***a2*** | 1.212 | 3.011 | 2.001 | 4.139 | 11.327 |
| | ***b1*** | 0.222 | 5.085 | 2.329 | 3.651 | 13.097 |
| | ***b2*** | 0.984 | 4.924 | 2.330 | 2.964 | 13.148 |

| | Substituent | Contribution of atoms (%) | | | | |
|---|---|---|---|---|---|---|
| | position | 6 | 7 | 8 | 9 | 10 |
| -$OCH_3$ | ***a1*** | 0.409 | 1.189 | 3.874 | 21.233 | 24.548 |
| | ***a2*** | 1.243 | 2.339 | 3.966 | 21.489 | 23.007 |
| | ***b1*** | 1.176 | 1.457 | 4.143 | 20.987 | 22.278 |
| | ***b2*** | 0.953 | 1.443 | 3.994 | 22.033 | 24.215 |
| -CHO | ***a1*** | 1.356 | 1.584 | 3.967 | 21.260 | 23.084 |
| | ***a2*** | 0.795 | 1.180 | 3.747 | 20.721 | 23.184 |
| | ***b1*** | 0.822 | 1.263 | 3.737 | 20.863 | 23.150 |
| | ***b2*** | 0.897 | 1.426 | 3.844 | 21.336 | 23.603 |
| -$NH_2$ | ***a1*** | 0.602 | 1.788 | 4.677 | 19.247 | 20.069 |
| | ***a2*** | 1.411 | 3.064 | 4.028 | 21.794 | 22.964 |
| | ***b1*** | 1.384 | 1.260 | 4.184 | 20.182 | 21.038 |
| | ***b2*** | 0.964 | 1.470 | 4.038 | 22.318 | 24.417 |
| -$NO_2$ | ***a1*** | 1.167 | 1.720 | 3.981 | 22.646 | 25.322 |
| | ***a2*** | 0.731 | 1.062 | 3.710 | 20.488 | 23.122 |
| | ***b1*** | 0.758 | 1.132 | 3.617 | 20.056 | 22.481 |
| | ***b2*** | 0.849 | 1.457 | 3.834 | 21.536 | 23.933 |
| -OH | ***a1*** | 0.605 | 1.593 | 4.919 | 18.622 | 18.220 |
| | ***a2*** | 1.171 | 2.236 | 3.973 | 21.855 | 23.583 |
| | ***b1*** | 1.824 | 1.194 | 4.441 | 18.241 | 17.914 |
| | ***b2*** | 0.933 | 1.415 | 3.970 | 21.919 | 24.140 |

**Section S7**. The energy (*E*), the squared eigenvalue of spin angular momentum (<$S^2$>), the magnetic coupling constant (*J*) and energy difference between SOMOs ($\Delta E_{SOMOs}$)

**Table S4.** The energy (*E*), the squared eigenvalue of spin angular momentum (<$S^2$>), the magnetic coupling constant (*J*) and energy difference between SOMOs ($\Delta E_{SOMOs}$) (B3LYP-D3/6-311G(d,p)).

| | **Substituent position** | $E_T$**/a.u.** ($< S^2 >_T$) | $E_{BS}$**/a.u.** ($< S^2 >_{BS}$) | $J$ **(cm$^{-1}$)** | $\Delta E_{SOMOs}$ **/(kcal/mol)** |
|---|---|---|---|---|---|
| origin | - | -1746.39084(2.032) | -1746.39047(0.962) | 75.46 | 17.344 |
| -$OCH_3$ | ***a1*** | -1860.94740(2.031) | -1860.94852(0.924) | -221.89 | 19.283 |
| | ***a2*** | -1860.95775(2.034) | -1860.95713(0.982) | 129.24 | 17.156 |
| | ***b1*** | -1860.96077(2.034) | -1860.95990(0.967) | 178.44 | 20.382 |
| | ***b2*** | -1860.95928(2.034) | -1860.95804(0.976) | 256.42 | 17.727 |
| -CHO | ***a1*** | -1859.74382(2.034) | -1859.74186(0.997) | 416.28 | 17.231 |
| | ***a2*** | -1859.74677(2.032) | -1859.74665(0.953) | 24.21 | 16.460 |
| | ***b1*** | -1859.74628(2.031) | -1859.74643(0.951) | -31.86 | 16.604 |
| | ***b2*** | -1859.74683(2.031) | -1859.74691(0.957) | -17.78 | 17.664 |
| -$NH_2$ | ***a1*** | -1801.78207(2.032) | -1801.78602(0.831) | -720.74 | 26.694 |
| | ***a2*** | -1801.78050(2.033) | -1801.78015(0.987) | 73.86 | 18.599 |
| | ***b1*** | -1801.78413(2.036) | -1801.78375(0.949) | 75.23 | 22.264 |
| | ***b2*** | -1801.78210(2.035) | -1801.78039(0.985) | 356.95 | 17.508 |
| -$NO_2$ | ***a1*** | -1950.93331(2.033) | -1950.93141(1.004) | 403.59 | 17.037 |
| | ***a2*** | -1950.94656(2.034) | -1950.94615(0.959) | 85.34 | 15.456 |
| | ***b1*** | -1950.94429(2.032) | -1950.94480(0.950) | -102.86 | 15.048 |
| | ***b2*** | -1950.94600(2.031) | -1950.94613(0.960) | -27.19 | 17.558 |
| -OH | ***a1*** | -1821.64726(2.032) | -1821.65007(0.854) | -522.21 | 27.698 |
| | ***a2*** | -1821.64112(2.033) | -1821.64057(0.978) | 114.79 | 17.614 |
| | ***b1*** | -1821.64423(2.036) | -1821.64334(0.973) | 184.87 | 21.819 |
| | ***b2*** | -1821.64203(2.033) | -1821.64091(0.975) | 232.77 | 17.489 |

**Section S8**. The contribution of atoms to the composition of SOMO1

**Table S5.** The contribution of atoms to the composition of SOMO1 (B3LYP-D3/6-311G(d,p)).

| | **Substituent position** | **$C_a$(%)** | **$C_b$(%)** |
|---|---|---|---|
| origin | - | 8.317 | 7.630 |
| -$OCH_3$ | ***a1*** | 5.650 | 9.816 |
| | ***a2*** | 7.613 | 9.746 |
| | ***b1*** | 11.026 | 5.813 |
| | ***b2*** | 10.890 | 5.656 |
| -CHO | ***a1*** | 10.123 | 6.148 |
| | ***a2*** | 8.428 | 6.454 |
| | ***b1*** | 6.879 | 8.154 |
| | ***b2*** | 6.754 | 8.852 |
| -$NH_2$ | ***a1*** | 4.048 | 12.199 |
| | ***a2*** | 6.304 | 11.544 |
| | ***b1*** | 12.828 | 3.894 |
| | ***b2*** | 12.112 | 4.568 |
| -$NO_2$ | ***a1*** | 11.169 | 5.958 |
| | ***a2*** | 8.928 | 5.650 |
| | ***b1*** | 5.550 | 9.309 |
| | ***b2*** | 5.870 | 9.737 |
| -OH | ***a1*** | 6.391 | 10.521 |
| | ***a2*** | 7.800 | 9.464 |
| | ***b1*** | 12.043 | 5.708 |
| | ***b2*** | 10.322 | 6.147 |

**Section S9.** The internuclear distances of $C_a$-$C_b$

**Table S6.** The internuclear distances of $C_a$-$C_b$ (B3LYP-D3/6-311G(d,p)).

| | **Substituent position** | **Distance/ Å** |
|---|---|---|
| origin | - | 2.881 |
| -$OCH_3$ | ***a1*** | 2.886 |
| | ***a2*** | 2.884 |
| | ***b1*** | 2.903 |
| | ***b2*** | 2.889 |
| -CHO | ***a1*** | 2.905 |
| | ***a2*** | 2.897 |
| | ***b1*** | 2.876 |
| | ***b2*** | 2.897 |
| -$NH_2$ | ***a1*** | 2.892 |
| | ***a2*** | 2.888 |
| | ***b1*** | 2.918 |
| | ***b2*** | 2.894 |
| -$NO_2$ | ***a1*** | 2.905 |
| | ***a2*** | 2.911 |
| | ***b1*** | 2.891 |
| | ***b2*** | 2.920 |
| -OH | ***a1*** | 2.888 |
| | ***a2*** | 2.884 |
| | ***b1*** | 2.938 |
| | ***b2*** | 2.887 |

**Section S10.** Detailed results obtained through verification calculations

**Table S7.** The contribution of atoms to the composition of SOMO1 (M06-2x/def2-TZVP).

| | **Substituent position** | **$C_a$(%)** | **$C_b$(%)** |
|---|---|---|---|
| origin | - | 10.337 | 7.889 |
| -$OCH_3$ | ***a1*** | 7.253 | 11.225 |
| | ***a2*** | 8.223 | 10.957 |
| | ***b1*** | 13.812 | 4.771 |
| | ***b2*** | 13.987 | 4.634 |
| -CHO | ***a1*** | 12.885 | 5.434 |
| | ***a2*** | 11.293 | 6.146 |
| | ***b1*** | 8.577 | 9.151 |
| | ***b2*** | 7.985 | 10.042 |
| -$NH_2$ | ***a1*** | 4.121 | 14.498 |
| | ***a2*** | 5.560 | 13.964 |
| | ***b1*** | 15.941 | 2.699 |
| | ***b2*** | 15.607 | 3.129 |
| -$NO_2$ | ***a1*** | 14.087 | 4.986 |
| | ***a2*** | 12.496 | 4.810 |
| | ***b1*** | 6.656 | 11.096 |
| | ***b2*** | 6.622 | 11.414 |
| -OH | ***a1*** | 7.125 | 11.641 |
| | ***a2*** | 8.499 | 10.595 |
| | ***b1*** | 14.154 | 4.908 |
| | ***b2*** | 13.211 | 5.365 |

**Table S8.** The energy (*E*), the squared eigenvalue of spin angular momentum (<$S^2$>), the magnetic coupling constant (*J*) and energy difference between SOMOs ($\Delta E_{SOMOs}$) (M06-2x/def2-TZVP).

| | **Substituent position** | $E_T$**/a.u.** ($< S^2 >_T$) | $E_{BS}$**/a.u.** ($< S^2 >_{BS}$) | $J$ **(cm$^{-1}$)** | $\Delta E_{SOMOs}$ **/(kcal/mol)** |
|---|---|---|---|---|---|
| origin | - | -1745.67914(2.032) | -1745.67832(0.995) | 173.10 | 26.914 |
| -$OCH_3$ | ***a1*** | -1860.20053(2.029) | -1860.20079(0.986) | -54.84 | 30.830 |
| | ***a2*** | -1860.21096(2.033) | -1860.21024(1.005) | 153.53 | 27.554 |
| | ***b1*** | -1860.21336(2.036) | -1860.21200(0.998) | 288.00 | 29.738 |
| | ***b2*** | -1860.21311(2.037) | -1860.21129(1.005) | 387.19 | 27.071 |
| -CHO | ***a1*** | -1859.00095(2.037) | -1858.99872(1.010) | 476.20 | 27.811 |
| | ***a2*** | -1859.00419(2.034) | -1859.00338(0.993) | 170.65 | 26.023 |
| | ***b1*** | -1859.00345(2.031) | -1859.00308(0.991) | 77.15 | 26.889 |
| | ***b2*** | -1859.00388(2.031) | -1859.00359(0.995) | 61.90 | 27.548 |
| -$NH_2$ | ***a1*** | -1801.05191(2.033) | -1801.05459(0.945) | -540.92 | 37.569 |
| | ***a2*** | -1801.05171(2.033) | -1801.05145(1.012) | 56.13 | 29.298 |
| | ***b1*** | -1801.05560(2.039) | -1801.05417(0.999) | 301.82 | 30.754 |
| | ***b2*** | -1801.05419(2.041) | -1801.05183(1.011) | 502.23 | 26.424 |
| -$NO_2$ | ***a1*** | -1950.17418(2.036) | -1950.17200(1.015) | 470.31 | 27.774 |
| | ***a2*** | -1950.18716(2.036) | -1950.18597(0.996) | 251.11 | 24.724 |
| | ***b1*** | -1950.18465(2.031) | -1950.18488(0.990) | -48.26 | 25.458 |
| | ***b2*** | -1950.18601(2.032) | -1950.18594(0.996) | 15.80 | 27.265 |
| -OH | ***a1*** | -1820.91997(2.032) | -1820.92163(0.949) | -336.97 | 37.789 |
| | ***a2*** | -1820.91616(2.032) | -1820.91549(1.003) | 142.11 | 28.087 |
| | ***b1*** | -1820.91856(2.036) | -1820.91699(1.003) | 333.67 | 30.516 |
| | ***b2*** | -1820.91747(2.036) | -1820.91580(1.003) | 354.60 | 26.901 |

**Table S9.** When the introduced radical is -N(O)CH($CH_3$)$_2$, the energy (*E*), the squared eigenvalue of spin angular momentum (<$S^2$>) and the magnetic coupling constant (*J*) (B3LYP-D3/6-311G(d,p)).

| | **Substituent position** | $E_T$**/a.u.** ($< S^2 >_T$) | $E_{BS}$**/a.u.** ($< S^2 >_{BS}$) | $J$ **(cm$^{-1}$)** |
|---|---|---|---|---|
| origin | - | -1864.38838 (2.031) | -1864.38862 (0.936) | -48.63 |
| -$NH_2$ | ***a1*** | -1919.77875 (2.032) | -1919.78355 (0.801) | -856.06 |
| | ***b2*** | -1919.77910 (2.033) | -1919.77794 (0.967) | 239.92 |
| -$NO_2$ | ***a1*** | -2068.93183 (2.032) | -2068.93031 (0.993) | 321.18 |
| | ***b2*** | -2068.94412 (2.030) | -2068.94484 (0.935) | -143.99 |