**SUPPORTING INFORMATION**

**METHODOLOGY**

The geometries of ground-state and the lowest-lying triplet excited-state have been investigated by the DFT and the time-dependent DFT (TD-DFT) methods with Becke’s LYP (B3LYP) exchange-correlation functional with the double-ζ quality basis set: 6-31G\*\* [1] and LanL2DZ [2,3] respectively, in addition, one f-type polarization function (αf=0.938) [4] was augmented to the Ir atom [5-7]. And there were no symmetry constraints on these complexes. A relativistic effective core potential (ECP) for Ir atom replaces the inner core electrons leaving the outer layer [(5s2)(5p6)] electrons and the (5d6) valence electrons [3]. The basis sets were depicted as Ir (8s6p3d/3s3p2d), C, N, O, F (10s4p1d/3s2p1d), S,P (16s10p1d/4s3p1d) and H (4s/2s).This combination of basis set is adequate to describe the ground and excited state geometries of the Ir complexes, and it has been verified and discussed elsewhere [8,9].

The respective optimized geometries of ground and excited states and the spectrum data were associated with the polarized continuum model (PCM) in CH2Cl2 medias, with the default parameters embedded in Gaussian09 to obtain a valid approximation of chemical environment, which have been shown to provide accurate interpretation and predication for the transition metal complexes in numerous applications in our previous works [10-14]. The M062x functional together with the same basis set mentioned above were adopted to evaluate the emission nature [15]. Furthermore, the stable configurations of these complexes can be confirmed by frequency analysis, in which no imaginary frequency was found for all configurations at the energy minimal. All calculations have been performed with Gaussian09 suite of program with a tight self-consistent field convergence threshold for both gradient and wave function convergence [16].

Table S1. The frontier molecular orbital composited by fragments in the ground state for the complex **1**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **TFPz1** | **TFPz2** | **Py1** | **Py2** | **acac** | **assign** |
| L+4 | -1.35 | 0.00 | 0.19 | 0.19 | 0.27 | 0.27 | 0.06 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| L+3 | -1.36 | 0.00 | 0.11 | 0.11 | 0.30 | 0.30 | 0.17 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| L+2 | -1.72 | 0.00 | 0.00 | 0.00 | 0.37 | 0.37 | 0.14 | π\*[(Py1)+(Py2)+(acac)] |
| L+1 | -1.97 | 0.00 | 0.26 | 0.26 | 0.22 | 0.22 | 0.00 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)] |
| L | -1.98 | 0.00 | 0.11 | 0.11 | 0.27 | 0.27 | 0.20 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| H | -6.11 | 0.40 | 0.23 | 0.23 | 0.00 | 0.00 | 0.05 | d(Ir)+π[(TFPz1)+(TFPz2)+(acac)] |
| H-1 | -6.45 | 0.15 | 0.17 | 0.17 | 0.14 | 0.14 | 0.00 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)] |
| H-2 | -6.63 | 0.00 | 0.19 | 0.19 | 0.27 | 0.27 | 0.06 | π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| H-3 | -6.70 | 0.13 | 0.21 | 0.21 | 0.10 | 0.10 | 0.25 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| H-4 | -7.26 | 0.35 | 0.16 | 0.16 | 0.14 | 0.14 | 0.05 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |
| H-5 | -7.34 | 0.09 | 0.33 | 0.33 | 0.00 | 0.00 | 0.18 | d(Ir)+π[(TFPz1)+(TFPz2)+(acac)] |
| H-6 | -7.53 | 0.22 | 0.16 | 0.16 | 0.08 | 0.08 | 0.31 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(acac)] |

Table S2. The frontier molecular orbital composited by fragments in the ground state for the complex **2**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **TFPz1** | **TFPz2** | **Py1** | **Py2** | **tpip** | **assign** |
| L+5 | -1.35 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.84 | π\*(tpip) |
| L+4 | -1.36 | 0.00 | 0.00 | 0.00 | 0.10 | 0.10 | 0.72 | π\*[(Py1)+(Py2)+(tpip)] |
| L+3 | -1.39 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.90 | π\*(tpip) |
| L+2 | -1.43 | 0.00 | 0.00 | 0.00 | 0.08 | 0.08 | 0.80 | π\*[(Py1)+(Py2)+(tpip)] |
| L+1 | -1.97 | 0.00 | 0.08 | 0.08 | 0.09 | 0.09 | 0.66 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| L | -1.99 | 0.00 | 0.10 | 0.10 | 0.06 | 0.06 | 0.65 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| H | -6.06 | 0.23 | 0.09 | 0.09 | 0.07 | 0.07 | 0.45 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| H-1 | -6.56 | 0.09 | 0.09 | 0.09 | 0.10 | 0.10 | 0.51 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| H-2 | -6.67 | 0.06 | 0.12 | 0.12 | 0.11 | 0.11 | 0.48 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| H-3 | -6.82 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.88 | π(tpip) |
| H-4 | -6.90 | 0.07 | 0.06 | 0.06 | 0.06 | 0.06 | 0.69 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |
| H-5 | -7.02 | 0.00 | 0.07 | 0.07 | 0.00 | 0.00 | 0.77 | π[(TFPz1)+(TFPz2)+(tpip)] |
| H-6 | -7.19 | 0.00 | 0.00 | 0.00 | 0.14 | 0.14 | 0.62 | π[(Py1)+(Py2)+(tpip)] |
| H-7 | -7.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.88 | π(tpip |
| H-8 | -7.28 | 0.00 | 0.07 | 0.07 | 0.26 | 0.26 | 0.33 | π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(tpip)] |

Table S3. The frontier molecular orbital composited by fragments in the ground state for the complex **3**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **TFPz1** | **TFPz2** | **Py1** | **Py2** | **dfbdp** | **assign** |
| L+3 | -1.36 | 0.00 | 0.08 | 0.09 | 0.12 | 0.16 | 0.51 | π\*[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(dfbdp)] |
| L+2 | -1.41 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.89 | π\*(dfbdp) |
| L+1 | -1.89 | 0.00 | 0.00 | 0.15 | 0.00 | 0.21 | 0.53 | π\*[(TFPz2)+(Py2)+(dfbdp)] |
| L | -1.98 | 0.00 | 0.05 | 0.14 | 0.10 | 0.00 | 0.63 | π\*[(TFPz1)+(TFPz2)+(Py1)+(dfbdp)] |
| H | -6.28 | 0.06 | 0.09 | 0.15 | 0.10 | 0.07 | 0.54 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(dfbdp)] |
| H-1 | -6.38 | 0.11 | 0.10 | 0.00 | 0.12 | 0.12 | 0.52 | d(Ir)+π[(TFPz1)+(Py1)+(Py2)+(dfbdp)] |
| H-2 | -6.53 | 0.10 | 0.08 | 0.18 | 0.00 | 0.10 | 0.50 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py2)+(dfbdp)] |
| H-3 | -6.64 | 0.11 | 0.10 | 0.10 | 0.14 | 0.05 | 0.50 | d(Ir)+π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(dfbdp)] |
| H-4 | -6.78 | 0.00 | 0.15 | 0.09 | 0.07 | 0.14 | 0.52 | π[(TFPz1)+(TFPz2)+(Py1)+(Py2)+(dfbdp)] |

Table S4. The frontier molecular orbital composited by fragments in the ground state for the complex **4**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **FPz1** | **FPz2** | **Py1** | **Py2** | **acac** | **assign** |
| L+3 | -1.30 | 0.00 | 0.08 | 0.08 | 0.34 | 0.34 | 0.15 | π\*[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| L+2 | -1.67 | 0.00 | 0.06 | 0.06 | 0.37 | 0.37 | 0.13 | π\*[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| L+1 | -1.91 | 0.00 | 0.17 | 0.17 | 0.26 | 0.26 | 0.10 | π\*[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| L | -1.92 | 0.06 | 0.00 | 0.00 | 0.25 | 0.25 | 0.35 | d(Ir)+π\*[(Py1)+(Py2)+(acac)] |
| H | -5.74 | 0.23 | 0.21 | 0.21 | 0.12 | 0.12 | 0.10 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| H-1 | -6.34 | 0.13 | 0.23 | 0.23 | 0.13 | 0.13 | 0.15 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| H-2 | -6.46 | 0.08 | 0.16 | 0.16 | 0.21 | 0.21 | 0.17 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| H-3 | -6.57 | 0.09 | 0.20 | 0.20 | 0.20 | 0.20 | 0.12 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| H-4 | -6.85 | 0.00 | 0.26 | 0.26 | 0.13 | 0.13 | 0.20 | π[(FPz1)+(FPz2)+(Py1)+(Py2)+(acac)] |
| H-5 | -7.16 | 0.33 | 0.10 | 0.10 | 0.21 | 0.21 | 0.00 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)] |

Table S5. The frontier molecular orbital composited by fragments in the ground state for the complex **5**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **FPz1** | **FPz2** | **Py1** | **Py2** | **tpip** | **assign** |
| L+5 | -1.23 | 0.00 | 0.00 | 0.00 | 0.12 | 0.00 | 0.83 | π\*[(Py1)+(tpip)] |
| L+4 | -1.23 | 0.00 | 0.00 | 0.00 | 0.00 | 0.20 | 0.66 | π\*[(Py2)+(tpip)] |
| L+3 | -1.31 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.91 | π\*(tpip) |
| L+2 | -1.34 | 0.00 | 0.00 | 0.00 | 0.07 | 0.06 | 0.78 | π\*[(Py1)+(Py2)+(tpip)] |
| L+1 | -1.85 | 0.00 | 0.08 | 0.08 | 0.13 | 0.12 | 0.56 | π\*[(FPz1)+(FPz2)+(Py1)+(Py2)+(tpip)] |
| L | -1.87 | 0.09 | 0.06 | 0.06 | 0.10 | 0.11 | 0.57 | d(Ir)+π\*[(FPz1)+(FPz2)+(Py1)+(Py2)+(tpip)] |
| H | -5.67 | 0.11 | 0.11 | 0.11 | 0.00 | 0.00 | 0.63 | d(Ir)+π[(FPz1)+(FPz2)+(tpip)] |
| H-1 | -6.34 | 0.06 | 0.15 | 0.16 | 0.25 | 0.25 | 0.13 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(tpip)] |
| H-2 | -6.51 | 0.05 | 0.06 | 0.06 | 0.17 | 0.17 | 0.49 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(tpip)] |
| H-3 | -6.65 | 0.11 | 0.07 | 0.07 | 0.00 | 0.00 | 0.66 | d(Ir)+π[(FPz1)+(FPz2)+(tpip)] |
| H-4 | -6.78 | 0.18 | 0.00 | 0.00 | 0.18 | 0.18 | 0.39 | d(Ir)+π[(Py1)+(Py2)+(tpip)] |
| H-5 | -6.83 | 0.00 | 0.12 | 0.11 | 0.00 | 0.00 | 0.68 | π[(FPz1)+(FPz2)+(tpip)] |
| H-6 | -6.93 | 0.06 | 0.09 | 0.09 | 0.17 | 0.17 | 0.42 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(tpip)] |

Table S6. The frontier molecular orbital composited by fragments in the ground state for the complex **6**.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **MO** | **Energy** | **Contribution** | | | | | | |
| **Ir** | **FPz1** | **FPz2** | **Py1** | **Py2** | **dfbdp** | **assign** |
| L+5 | -1.18 | 0.00 | 0.29 | 0.00 | 0.11 | 0.00 | 0.52 | π\*[(FPz1)+(Py1)+(dfbdp)] |
| L+4 | -1.24 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.93 | π\*[(dfbdp)] |
| L+3 | -1.30 | 0.00 | 0.00 | 0.06 | 0.07 | 0.06 | 0.66 | π\*[(FPz2)+(Py1)+(Py2)+(dfbdp)] |
| L+2 | -1.35 | 0.00 | 0.00 | 0.00 | 0.05 | 0.00 | 0.86 | π\*[(Py1)+(dfbdp)] |
| L+1 | -1.83 | 0.07 | 0.00 | 0.06 | 0.06 | 0.28 | 0.52 | d(Ir)+π\*[(FPz2)+(Py1)+(Py2)+(dfbdp)] |
| L | -1.92 | 0.00 | 0.00 | 0.00 | 13.00 | 0.00 | 0.68 | π\*[(Py1)+(dfbdp)] |
| H | -5.92 | 0.05 | 0.06 | 0.16 | 0.11 | 0.07 | 0.55 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(dfbdp)] |
| H-1 | -6.24 | 0.00 | 0.07 | 0.10 | 0.08 | 0.26 | 0.46 | π[(FPz1)+(FPz2)+(Py1)+(Py2)+(dfbdp)] |
| H-2 | -6.36 | 0.12 | 0.09 | 0.20 | 0.00 | 0.07 | 0.48 | d(Ir)+π[(FPz1)+(FPz2)+(Py2)+(dfbdp)] |
| H-3 | -6.51 | 0.09 | 0.13 | 0.07 | 0.29 | 0.08 | 0.35 | d(Ir)+π[(FPz1)+(FPz2)+(Py1)+(Py2)+(dfbdp)] |

Table S7. Calculated absorptions of complexes 1–6 in CH2Cl2 media.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Complex** | **States** | **Energy(nm/eV)** | **Oscillator** | **Main Configurations** | **Assign** |
| 1 | S1 | 369/3.36 | 0.054 | HOMO→LUMO+1(70%) | TFPz1/TFPz2/acac→TFPz1/TFPz2/Py1/Py2 |
|  | S12 | 298/4.16 | 0.130 | HOMO-3→LUMO+1(65%) | TFPz1/TFPz2/Py1/Py2/acac→TFPz1/TFPz2/Py1/Py2 |
| S19 | 277/4.47 | 0.118 | HOMO-4→LUMO+1(50%) | TFPz1/TFPz2/Py1/Py2/acac→TFPz1/TFPz2/Py1/Py2 |
|  |  |  | HOMO-1→LUMO+3(41%) | TFPz1/TFPz2/Py1/Py2→TFPz1/TFPz2/Py1/Py2/acac |
| S25 | 262/4.73 | 0.175 | HOMO-5→LUMO(53%) | TFPz1/TFPz2/acac→TFPz1/TFPz2/Py1/Py2/acac |
|  |  |  | HOMO-2→LUMO+3(34%) | TFPz1/TFPz2/Py1/Py2/acac→TFPz1/TFPz2/Py1/Py2/acac |
| S30 | 252/4.91 | 0.383 | HOMO-6→LUMO(55%) | TFPz1/TFPz2/Py1/Py2/acac→TFPz1/TFPz2/Py1/Py2/acac |
|  |  |  | HOMO-3→LUMO+4(28%) | TFPz1/TFPz2/Py1/Py2/acac→TFPz1/TFPz2/Py1/Py2/acac |
| 2 | S1 | 379/3.27 | 0.041 | HOMO→LUMO(69%) | TFPz1/TFPz2/Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
|  | S9 | 305/4.07 | 0.083 | HOMO-2→LUMO+1(46%) | TFPz1/TFPz2/Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
|  |  |  | HOMO-1→LUMO(29%) | TFPz1/TFPz2/Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
| S12 | 297/4.17 | 0.096 | HOMO-3→LUMO+1(56%) | tpip→TFPz1/TFPz2/Py1/Py2/tpip |
|  |  |  | HOMO-1→LUMO+1(31%) | TFPz1/TFPz2/Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
| S22 | 269/4.62 | 0.168 | HOMO-1→LUMO+5(44%) | TFPz1/TFPz2/Py1/Py2/tpip→tpip |
|  |  |  | HOMO-1→LUMO+3(35%) | TFPz1/TFPz2/Py1/Py2/tpip→tpip |
| S30 | 263/4.71 | 0.098 | HOMO-8→LUMO(33%) | TFPz1/TFPz2/Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
|  |  |  | HOMO-6→LUMO(31%) | Py1/Py2/tpip→TFPz1/TFPz2/Py1/Py2/tpip |
| 3 | S1 | 346/3.58 | 0.050 | HOMO→LUMO(65%) | TFPz1/TFPz2/Py1/Py2/dfbdp→TFPz1/TFPz2/Py1/dfbdp |
|  | S6 | 305/4.06 | 0.125 | HOMO-2→LUMO+1(66%) | TFPz1/TFPz2/Py2/dfbdp→TFPz2/Py2/dfbdp |
| S7 | 305/4.07 | 0.099 | HOMO-3→LUMO(66%) | TFPz1/TFPz2/Py1/Py2/dfbdp→TFPz1/TFPz2/Py1/dfbdp |
| S16 | 282/4.40 | 0.108 | HOMO-1→LUMO+3(59%) | TFPz1/Py1/Py2/dfbdp→TFPz1/TFPz2/Py1/Py2/dfbdp |
|  |  |  | HOMO-4→LUMO(23%) | TFPz1/TFPz2/Py1/Py2/dfbdp→TFPz1/TFPz2/Py1/dfbdp |
| 4 | S1 | 402/3.09 | 0.06 | HOMO→LUMO+1(70%) | FPz1/FPz2/Py1/Py2/acac→FPz1/FPz2/Py1/Py2/acac |
|  | S10 | 315/3.93 | 0.100 | HOMO-2→LUMO(59%) | FPz1/FPz2/Py1/Py2/acac→Py1/Py2/acac |
|  |  |  | HOMO-1→LUMO(33%) | FPz1/FPz2/Py1/Py2/acac→Py1/Py2/acac |
| S12 | 303/4.09 | 0.133 | HOMO-3→LUMO+1(67%) | FPz1/FPz2/Py1/Py2/acac→FPz1/FPz2/Py1/Py2/acac |
| S21 | 280/4.44 | 0.114 | HOMO-5→LUMO+1(43%) | FPz1/FPz2/Py1/Py2→FPz1/FPz2/Py1/Py2/acac |
|  |  |  | HOMO-2→LUMO+3(37%) | FPz1/FPz2/Py1/Py2/acac→FPz1/FPz2/Py1/Py2/acac |
| S24 | 270/4.59 | 0.180 | HOMO-2→LUMO+3(57%) | FPz1/FPz2/Py1/Py2/acac→FPz1/FPz2/Py1/Py2/acac |
|  |  |  | HOMO-1→LUMO+3(33%) | FPz1/FPz2/Py1/Py2/acac→FPz1/FPz2/Py1/Py2/acac |
| 5 | S1 | 408/3.04 | 0.049 | HOMO→LUMO | FPz1/FPz2/tpip→FPz1/FPz2/Py1/Py2/tpip |
|  | S12 | 305/4.06 | 0.074 | HOMO-3→LUMO+1(59%) | FPz1/FPz2/tpip→FPz1/FPz2/Py1/Py2/tpip |
|  |  |  | HOMO-1→LUMO+1(26%) | FPz1/FPz2/Py1/Py2/tpip→FPz1/FPz2/Py1/Py2/tpip |
| S15 | 297/4.18 | 0.097 | HOMO-4→LUMO(53%) | Py1/Py2/tpip→FPz1/FPz2/Py1/Py2/tpip |
|  |  |  | HOMO-2→LUMO(35%) | FPz1/FPz2/Py1/Py2/tpip→FPz1/FPz2/Py1/Py2/tpip |
| S26 | 272/4.55 | 0.133 | HOMO-1→LUMO+3(57%) | FPz1/FPz2/Py1/Py2/tpip→tpip |
|  |  |  | HOMO-6→LUMO+1(21%) | FPz1/FPz2/Py1/Py2/tpip→FPz1/FPz2/Py1/Py2/tpip |
| S27 | 270/4.59 | 0.076 | HOMO-1→LUMO+5(44%) | FPz1/FPz2/Py1/Py2/tpip→Py1/tpip |
|  |  |  | HOMO-1→LUMO+4(30%) | FPz1/FPz2/Py1/Py2/tpip→Py2/tpip |
| 6 | S1 | 375/3.30 | 0.048 | HOMO→LUMO(69%) | FPz1/FPz2/Py1/Py2/dfbdp→Py1/dfbdp |
|  | S7 | 316/3.92 | 0.063 | HOMO-2→LUMO+1(49%) | FPz1/FPz2/Py2/dfbdp→FPz2/Py1/Py2/dfbdp |
|  |  |  | HOMO→LUMO+2(28%) | FPz1/FPz2/Py1/Py2/dfbdp→Py1/dfbdp |
| S10 | 309/4.02 | 0.057 | HOMO-3→LUMO(40%) | FPz1/FPz2/Py1/Py2/dfbdp→Py1/dfbdp |
|  |  |  | HOMO→LUMO+5(35%) | FPz1/FPz2/Py1/Py2/dfbdp→FPz1/Py1/dfbdp |
| S11 | 303/4.09 | 0.081 | HOMO-3→LUMO+1(67%) | FPz1/FPz2/Py1/Py2/dfbdp→FPz2/Py1/Py2/dfbdp |
| S19 | 284/4.37 | 0.131 | HOMO-1→LUMO+3(44%) | FPz1/FPz2/Py1/Py2/dfbdp→FPz2/Py1/Py2/dfbdp |
|  |  |  | HOMO-1→LUMO+2(35%) | FPz1/FPz2/Py1/Py2/dfbdp→Py1/dfbdp |



Figure A. The optimized ground-state geometrical structures for the complex **1～6.**

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