Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## A theoretical study on the electronic and photophysical properties of two series of iridium(III) complexes with different substituted N^N ligand†

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**Table S1** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **1**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | pyrapy | mbiphpyrapy | |
| L+8 | -2.31 | 2 | 12 | 8 | 78 | π*( mbiphpyrapy) |
| L+7 | -2.68 | 1 | 4 | 78 | 17 | π*( pyrapy) |
| L+6 | -2.88 | 0 | 5 | 8 | 87 | π*( mbiphpyrapy) |
| L+5 | -3.24 | 2 | 95 | 1 | 3 | π*( C^N) |
| L+4 | -3.35 | 2 | 91 | 6 | 1 | π*( C^N) |
| L+3 | -3.82 | 1 | 16 | 83 | 0 | π*( C^N+ pyrapy) |
| L+2 | -3.87 | 4 | 87 | 9 | 1 | π*(C^N) |
| L+1 | -4.01 | 5 | 92 | 3 | 0 | π*( C^N) |
| L | -4.56 | 3 | 2 | 95 | 1 | π*( pyrapy) |
| H | -7.41 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-1 | -8.14 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-2 | -8.18 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-3 | -8.34 | 0 | 2 | 0 | 97 | π(mbiphpyrapy) |
| H-4 | -8.47 | 31 | 66 | 1 | 1 | d(Ir)+π(C^N) |
| H-5 | -8.81 | 4 | 91 | 1 | 5 | π(C^N) |
| H-6 | -8.85 | 0 | 3 | 0 | 97 | π(mbiphpyrapy) |
| H-7 | -8.91 | 8 | 89 | 1 | 3 | π(C^N) |
| H-8 | -8.98 | 0 | 0 | 0 | 99 | π(mbiphpyrapy) |

**Table S2** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **1a**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | pyrapy | mbiphpyrapy | |
| L+8 | -2.26 | 1 | 3 | 8 | 87 | π*( mbiphpyrapy) |
| L+7 | -2.60 | 1 | 2 | 81 | 15 | π*( pyrapy) |
| L+6 | -2.85 | 0 | 6 | 4 | 89 | π*( mbiphpyrapy) |
| L+5 | -3.22 | 2 | 94 | 0 | 4 | π*( C^N) |
| L+4 | -3.34 | 2 | 88 | 9 | 1 | π*( C^N) |
| L+3 | -3.73 | 1 | 26 | 73 | 0 | π*( C^N+ pyrapy) |
| L+2 | -3.77 | 4 | 80 | 16 | 1 | π*( C^N+ pyrapy) |
| L+1 | -3.91 | 5 | 91 | 4 | 0 | π*( C^N) |
| L | -4.46 | 3 | 2 | 95 | 1 | π*( pyrapy) |
| H | -7.40 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-1 | -8.14 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-2 | -8.19 | 0 | 0 | 0 | 99 | π(mbiphpyrapy) |
| H-3 | -8.24 | 28 | 68 | 1 | 3 | d(Ir)+π(C^N) |
| H-4 | -8.33 | 1 | 2 | 0 | 96 | π(mbiphpyrapy) |
| H-5 | -8.61 | 3 | 95 | 0 | 1 | π(C^N) |
| H-6 | -8.85 | 0 | 2 | 0 | 97 | π(mbiphpyrapy) |
| H-7 | -8.88 | 14 | 79 | 1 | 6 | d(Ir)+π(C^N) |
| H-8 | -8.99 | 0 | 0 | 0 | 99 | π(mbiphpyrapy) |

**Table S3** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **1b**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | $CF_3$-pyrapy | mbiphpyrapy | |
| L+8 | -2.35 | 1 | 5 | 5 | 89 | π*( mbiphpyrapy) |
| L+7 | -2.76 | 1 | 2 | 79 | 17 | π*($CF_3$-pyrapy+mbiphpyrapy) |
| L+6 | -2.92 | 1 | 6 | 9 | 84 | π*( mbiphpyrapy) |
| L+5 | -3.31 | 2 | 94 | 0 | 4 | π*( C^N) |
| L+4 | -3.45 | 2 | 93 | 4 | 1 | π*( C^N) |
| L+3 | -3.85 | 4 | 94 | 1 | 1 | π*( C^N) |
| L+2 | -3.99 | 4 | 86 | 10 | 0 | π*(C^N) |
| L+1 | -4.11 | 2 | 11 | 87 | 0 | π*($CF_3$-pyrapy) |
| L | -4.81 | 3 | 1 | 95 | 1 | π*($CF_3$-pyrapy) |
| H | -7.43 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-1 | -8.17 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-2 | -8.22 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-3 | -8.34 | 24 | 63 | 1 | 13 | d(Ir)+π(C^N) |
| H-4 | -8.39 | 4 | 10 | 0 | 86 | π(mbiphpyrapy) |
| H-5 | -8.71 | 3 | 95 | 0 | 1 | π(C^N) |
| H-6 | -8.88 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-7 | -8.98 | 13 | 82 | 1 | 3 | d(Ir)+π(C^N) |
| H-8 | -9.03 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |

**Table S4** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **1c**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | $CF_3$-pyrapy | mbiphpyrapy | |
| L+8 | -2.40 | 4 | 20 | 6 | 71 | π*(C^N+mbiphpyrapy) |
| L+7 | -2.82 | 1 | 2 | 70 | 26 | π*($CF_3$-pyrapy+mbiphpyrapy) |
| L+6 | -2.96 | 1 | 5 | 18 | 76 | π*($CF_3$-pyrapy+mbiphpyrapy) |
| L+5 | -3.33 | 2 | 95 | 1 | 3 | π*( C^N) |
| L+4 | -3.45 | 2 | 94 | 4 | 1 | π*( C^N) |
| L+3 | -3.96 | 4 | 94 | 1 | 1 | π*( C^N) |
| L+2 | -4.10 | 4 | 85 | 10 | 0 | π*(C^N) |
| L+1 | -4.19 | 2 | 11 | 87 | 0 | π*( $CF_3$-pyrapy) |
| L | -4.90 | 3 | 1 | 95 | 1 | π*( $CF_3$-pyrapy) |
| H | -7.44 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-1 | -8.16 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-2 | -8.21 | 0 | 0 | 0 | 100 | π(mbiphpyrapy) |
| H-3 | -8.38 | 0 | 2 | 0 | 98 | π(mbiphpyrapy) |
| H-4 | -8.57 | 30 | 68 | 1 | 1 | d(Ir)+π(C^N) |
| H-5 | -8.87 | 0 | 3 | 0 | 96 | π(mbiphpyrapy) |
| H-6 | -8.90 | 4 | 90 | 0 | 6 | π(C^N) |
| H-7 | -9.01 | 8 | 88 | 1 | 4 | π(C^N) |
| H-8 | -9.02 | 0 | 2 | 0 | 98 | π(mbiphpyrapy) |

**Table S5** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **2**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | triapy | mphtriapy | |
| L+8 | -2.96 | 0 | 1 | 2 | 97 | π*( mphtriapy) |
| L+7 | -2.97 | 0 | 5 | 7 | 88 | π*( mphtriapy) |
| L+6 | -3.08 | 2 | 91 | 3 | 4 | π*(C^N) |
| L+5 | -3.16 | 0 | 2 | 6 | 92 | π*( mphtriapy) |
| L+4 | -3.35 | 1 | 11 | 78 | 11 | π*( triapy) |
| L+3 | -3.49 | 4 | 86 | 8 | 2 | π*( C^N) |
| L+2 | -3.74 | 4 | 84 | 11 | 1 | π*(C^N) |
| L+1 | -3.75 | 2 | 13 | 81 | 3 | π*( triapy) |
| L | -4.35 | 2 | 0 | 96 | 1 | π*( triapy) |
| H | -8.09 | 29 | 69 | 1 | 0 | d(Ir)+π(C^N) |
| H-1 | -8.43 | 6 | 93 | 0 | 0 | π(C^N) |
| H-2 | -8.62 | 5 | 94 | 0 | 0 | π(C^N) |
| H-3 | -8.92 | 3 | 96 | 1 | 0 | π(C^N) |
| H-4 | -9.00 | 1 | 0 | 0 | 99 | π(mphtriapy) |
| H-5 | -9.07 | 68 | 26 | 5 | 1 | d(Ir)+π(C^N) |
| H-6 | -9.18 | 66 | 26 | 8 | 1 | d(Ir)+π(C^N) |
| H-7 | -9.71 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-8 | -9.84 | 0 | 0 | 5 | 95 | π(mphtriapy) |

**Table S6** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **2a**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | triapy | mphtriapy | |
| L+8 | -2.82 | 0 | 1 | 17 | 81 | π*(triapy+mphtriapy) |
| L+7 | -2.94 | 2 | 94 | 1 | 4 | π*( C^N) |
| L+6 | -2.98 | 0 | 5 | 2 | 93 | π*( mphtriapy) |
| L+5 | -3.03 | 2 | 79 | 8 | 11 | π*( C^N) |
| L+4 | -3.13 | 1 | 5 | 60 | 35 | π*( triapy+mphtriapy) |
| L+3 | -3.46 | 3 | 46 | 50 | 1 | π*( C^N+ triapy) |
| L+2 | -3.50 | 3 | 61 | 36 | 1 | π*( C^N+ triapy) |
| L+1 | -3.60 | 5 | 93 | 2 | 0 | π*( C^N) |
| L | -4.09 | 3 | 2 | 96 | 0 | π*( triapy) |
| H | -7.86 | 29 | 70 | 1 | 0 | d(Ir)+π(C^N) |
| H-1 | -8.29 | 4 | 95 | 0 | 0 | π(C^N) |
| H-2 | -8.55 | 11 | 89 | 1 | 0 | π(C^N) |
| H-3 | -8.70 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-4 | -8.89 | 23 | 73 | 4 | 0 | d(Ir)+π(C^N) |
| H-5 | -8.92 | 68 | 25 | 6 | 0 | d(Ir)+π(C^N) |
| H-6 | -9.02 | 47 | 47 | 6 | 0 | d(Ir)+π(C^N) |
| H-7 | -9.32 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-8 | -9.73 | 1 | 2 | 86 | 11 | π(triapy) |

**Table S7** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **2b**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | $CF_3$-triapy | mphtriapy | |
| L+8 | -2.89 | 1 | 2 | 18 | 79 | π*($CF_3$-triapy+mphtriapy) |
| L+7 | -2.99 | 0 | 0 | 2 | 97 | π*( mphtriapy) |
| L+6 | -3.06 | 2 | 96 | 1 | 2 | π*(C^N) |
| L+5 | -3.14 | 2 | 74 | 15 | 9 | π*(C^N) |
| L+4 | -3.28 | 1 | 22 | 63 | 13 | π*( C^N+ $CF_3$-triapy) |
| L+3 | -3.60 | 4 | 95 | 1 | 0 | π*( C^N) |
| L+2 | -3.72 | 4 | 94 | 2 | 0 | π*(C^N) |
| L+1 | -3.88 | 1 | 5 | 94 | 1 | π*( $CF_3$-triapy) |
| L | -4.52 | 3 | 0 | 96 | 0 | π*( $CF_3$-triapy) |
| H | -8.00 | 28 | 71 | 1 | 0 | d(Ir)+π(C^N) |
| H-1 | -8.41 | 4 | 96 | 0 | 0 | π(C^N) |
| H-2 | -8.51 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-3 | -8.67 | 10 | 89 | 1 | 0 | π(C^N) |
| H-4 | -9.02 | 14 | 82 | 3 | 0 | π(C^N) |
| H-5 | -9.08 | 69 | 25 | 6 | 0 | d(Ir)+π(C^N) |
| H-6 | -9.13 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-7 | -9.18 | 56 | 38 | 7 | 0 | d(Ir)+π(C^N) |
| H-8 | -9.73 | 0 | 0 | 0 | 100 | π(mphtriapy) |

**Table S8** Frontier molecular orbital energies (eV) and compositions (%) in the ground state for complex **2c**

| MO | Energy | Contribution (%) | | | | Assignment |
|---|---|---|---|---|---|---|
| | | Ir | C^N | $CF_3$-triapy | mphtriapy | |
| L+8 | -2.94 | 0 | 2 | 17 | 80 | π*($CF_3$-triapy+mphtriapy) |
| L+7 | -3.03 | 0 | 0 | 2 | 97 | π*( mphtriapy) |
| L+6 | -3.09 | 2 | 96 | 0 | 2 | π*(C^N) |
| L+5 | -3.16 | 2 | 86 | 7 | 5 | π*(C^N) |
| L+4 | -3.35 | 1 | 11 | 73 | 15 | π*( $CF_3$-triapy+ mphtriapy) |
| L+3 | -3.71 | 4 | 94 | 2 | 0 | π*(C^N) |
| L+2 | -3.83 | 4 | 93 | 2 | 0 | π*(C^N) |
| L+1 | -3.98 | 1 | 5 | 94 | 1 | π*( $CF_3$-triapy) |
| L | -4.62 | 3 | 0 | 96 | 0 | π*( $CF_3$-triapy) |
| H | -8.22 | 30 | 68 | 1 | 0 | d(Ir)+π(C^N) |
| H-1 | -8.54 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-2 | -8.59 | 5 | 95 | 0 | 0 | π(C^N) |
| H-3 | -8.72 | 5 | 95 | 0 | 0 | π(C^N) |
| H-4 | -9.04 | 3 | 95 | 1 | 0 | π(C^N) |
| H-5 | -9.16 | 0 | 0 | 0 | 100 | π(mphtriapy) |
| H-6 | -9.22 | 69 | 24 | 6 | 0 | d(Ir)+π(C^N) |
| H-7 | -9.31 | 65 | 26 | 8 | 0 | d(Ir)+π(C^N) |
| H-8 | -9.77 | 0 | 0 | 0 | 100 | π(mphtriapy) |

**Table S9** Selected calculated wavelength (nm)/energies (eV), oscillator strength (*f*), major contribution and transition characters for **1-1c** in $CH_2Cl_2$ media, along with the experimental data for **1**

| | State | λ/E | *f* | Configuration | Assignment | Exptl[a] |
|---|---|---|---|---|---|---|
| **1** | $S_1$ | 366/3.38 | 0.002 | H→L(96%) | [π(mbiphpyrapy)→π*( pyrapy)] ILCT | 363 |
| | $S_{22}$ | 277/4.47 | 0.195 | H→L+4(65%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{27}$ | 269/4.59 | 0.743 | H-7→L (56%) | [π(C^N)→π*( pyrapy)] LLCT | |
| | $S_{31}$ | 263/4.70 | 0.339 | H-1→L+6 (79%) | [π(mbiphpyrapy)→π*(mbiphpyrapy)] ILCT | |
| | $S_{40}$ | 252/4.91 | 0.176 | H-1→L+7(58%) | [π(mbiphpyrapy)→π*( pyrapy)] ILCT | |
| | $S_{44}$ | 251/4.93 | 0.205 | H-5→L+3(50%) | [π(C^N)→π*( C^N+ pyrapy)] LLCT/ILCT | |
| | $S_{54}$ | 244/5.07 | 0.132 | H→L+5(49%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| **1a** | $S_1$ | 381/3.25 | 0.002 | H→L(97%) | [π(mbiphpyrapy)→π*( pyrapy)] ILCT | |
| | $S_{21}$ | 279/4.43 | 0.088 | H-6→L+2(51%) | [π(mbiphpyrapy)→π*(C^N+pyrapy)]LLCT /ILCT | |
| | $S_{26}$ | 270/4.58 | 0.263 | H→L+6(51%) | [π(mbiphpyrapy)→π*( mbiphpyrapy)] ILCT | |
| | $S_{31}$ | 263/4.71 | 0.405 | H-1→L+6(43%) | [π(mbiphpyrapy)→π*( mbiphpyrapy)] ILCT | |
| | $S_{36}$ | 257/4.81 | 0.128 | H-8→L(49%) | [π(mbiphpyrapy)→π*( pyrapy)] ILCT | |
| | $S_{42}$ | 251/4.92 | 0.173 | H-1→L+7 (47%) | [π(mbiphpyrapy)→π*( pyrapy)] ILCT | |
| | $S_{50}$ | 247/5.00 | 0.102 | H-1→L+4 (66%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| **1b** | $S_1$ | 417/2.96 | 0.002 | H→L(97%) | [π(mbiphpyrapy)→π*($CF_3$-pyrapy)] ILCT | |
| | $S_{27}$ | 275/4.49 | 0.152 | H-6→L (43%) | [π(mbiphpyrapy)→π*($CF_3$-pyrapy)] ILCT | |
| | $S_{34}$ | 267/4.63 | 0.441 | H-1→L+4 (56%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{38}$ | 263/4.70 | 0.206 | H-6→L+3 (66%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{43}$ | 257/4.82 | 0.236 | H-3→L+5(74%) | [d(Ir)+π(C^N)→π*( C^N)] MLCT/LLCT/ILCT | |
| | $S_{45}$ | 252/4.91 | 0.268 | H-1→L+7 (54%) | [π(mbiphpyrapy)→π*($CF_3$-pyrapy+mbiphpyrapy)] ILCT | |
| | $S_{54}$ | 247/5.01 | 0.128 | H→L+7 (46%) | [π(mbiphpyrapy)→π*($CF_3$-pyrapy+mbiphpyrapy)] ILCT | |
| **1c** | $S_1$ | 399/3.10 | 0.001 | H→L(73%) | [π(mbiphpyrapy)→π*( $CF_3$-pyrapy)] ILCT | |
| | $S_{25}$ | 277/4.46 | 0.178 | H-2→L+4 (61%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{28}$ | 275/4.50 | 0.170 | H-8→L+1 (49%) | [π(mbiphpyrapy)→π*( $CF_3$-pyrapy)] ILCT | |
| | $S_{35}$ | 267/4.63 | 0.667 | H-5→L+5 (55%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{39}$ | 262/4.73 | 0.261 | H-2→L+4 (51%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{45}$ | 252/4.91 | 0.416 | H-2→L+5 (45%) | [π(mbiphpyrapy)→π*( C^N)] LLCT | |
| | $S_{57}$ | 244/5.06 | 0.182 | H→L+8 (43%) | [π(mbiphpyrapy)→π*(C^N+mbiphpyrapy)] LLCT/ILCT | |

[a] From ref. 19

**Table S10** Selected calculated wavelength (nm)/energies (eV), oscillator strength (*f*), major contribution and transition characters for **2-2c** in $CH_2Cl_2$ media, along with the experimental data for **2**

| | State | λ/E | *f* | Configuration | Assignment | Exptl[a] |
|---|---|---|---|---|---|---|
| **2** | $S_1$ | 371/3.33 | 0.002 | H→L(96%) | [d(Ir)+π(C^N)→π*(triapy)]MLCT/LLCT | 361 |
| | $S_{12}$ | 293/4.22 | 0.170 | H-1→L+2 (73%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{18}$ | 278/4.45 | 0.100 | H-5→L+1(53%) | [d(Ir)+π(C^N)→π*( triapy)] MLCT/LLCT | |
| | $S_{28}$ | 260/4.75 | 0.084 | H-2→L+3 (45%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{34}$ | 251/4.92 | 0.100 | H-1→L+6(72%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{39}$ | 248/4.98 | 0.154 | H-2→L+6(60%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{44}$ | 244/5.07 | 0.123 | H-1→L+7 (48%) | [π(C^N)→π*( mphtriapy)] LLCT | |
| **2a** | $S_1$ | 378/3.27 | 0.001 | H→L(97%) | [d(Ir)+π(C^N)→π*( triapy)] MLCT/LLCT | |
| | $S_{10}$ | 295/4.18 | 0.083 | H-2→L+1(57%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{19}$ | 278/4.44 | 0.158 | H-5→L+2 (47%) | [d(Ir)+π(C^N)→π*( C^N+ triapy)] MLCT/LLCT/ILCT | |
| | $S_{27}$ | 259/4.76 | 0.114 | H-7→L(67%) | [π(mphtriapy)→π*( triapy)] ILCT | |
| | $S_{39}$ | 249/4.96 | 0.425 | H-3→L+4(45%) | [π(mphtriapy)→π*( triapy+mphtriapy)] ILCT | |
| | $S_{42}$ | 246/5.03 | 0.146 | H→L+8 (41%) | [d(Ir)+π(C^N)→π*(triapy+mphtriapy)] MLCT/LLCT | |
| | $S_{55}$ | 235/5.25 | 0.137 | H-5→L+7(60%) | [d(Ir)+π(C^N)→π*( C^N)] MLCT/LLCT /ILCT | |
| **2b** | $S_1$ | 420/2.94 | 0.001 | H→L(97%) | [d(Ir)+π(C^N)→π*( $CF_3$-triapy)] MLCT/LLCT | |
| | $S_8$ | 316/3.91 | 0.113 | H-5→L (70%) | [d(Ir)+π(C^N)→π*( $CF_3$-triapy)] MLCT/LLCT | |
| | $S_{23}$ | 276/4.48 | 0.143 | H-4→L+2(45%) | [π(C^N)→π*( C^N)] MLCT/LLCT/ILCT | |
| | $S_{28}$ | 263/4.71 | 0.108 | H-6→L+1(49%) | [π(mphtriapy)→π*( $CF_3$-triapy)] ILCT | |
| | $S_{35}$ | 256/4.84 | 0.256 | H-1→L+6 (45%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |
| | $S_{41}$ | 251/4.93 | 0.374 | H-2→L+5(70%) | [π(mphtriapy)→π*( C^N)] LLCT/ILCT | |
| | $S_{46}$ | 246/5.02 | 0.107 | H→L+2 (43%) | [d(Ir)+π(C^N)→π*(C^N)] MLCT/LLCT/ILCT | |
| **2c** | $S_1$ | 402/3.07 | 0.003 | H→L(97%) | [d(Ir)+π(C^N)→π*( $CF_3$-triapy)] MLCT/LLCT | |
| | $S_9$ | 311/3.98 | 0.139 | H-6→L (63%) | [d(Ir)+π(C^N)→π*( $CF_3$-triapy)] MLCT/LLCT | |
| | $S_{23}$ | 273/4.52 | 0.135 | H-4→L+2 (73%) | [π(C^N)→π*(C^N)] LLCT/ILCT | |
| | $S_{39}$ | 251/4.93 | 0.298 | H-2→L+5 (55%) | [π(C^N)→π*( C^N)] LLCT/ILCT | |

[a] From ref. 19

**Table S11** Calculated phosphorescent emission wavelength (λ, in nm) for **1** and **2** in $CH_2Cl_2$ media with the TDDFT method at M062X, M052X, PBE0, B3LYP, CAM-B3LYP and BP86 level, respectively, together with the experimental values

| | Exptl[a] | M062X | M052X | PBE0 | B3LYP | CAM-B3LYP | BP86 |
|---|---|---|---|---|---|---|---|
| 1 | 454 | 479 | 511 | 555 | 540 | 567 | 553 |
| 2 | 454 | 476 | 507 | 552 | 538 | 561 | 556 |

[a] From ref. 19

**Table S12** Frontier molecular orbital energies (eV) and composition (%) of **1-1c** and **2-2c** in the lowest lying triplet excited state (L and H represent)

| | MO | *E* | MO composition (%) | | | Assignment |
|---|---|---|---|---|---|---|
| **1** | | | Ir | C^N | N^N | |
| | L | -4.55 | 3 | 3 | 94 | π*( N^N) |
| | H | -7.40 | 0 | 0 | 100 | π(N^N) |
| **1a** | | | Ir | C^N | N^N | |
| | L | -4.88 | 4 | 1 | 95 | π*( N^N) |
| | H | -7.39 | 0 | 0 | 100 | π(N^N) |
| **1b** | | | Ir | C^N | N^N | |
| | L | -5.26 | 4 | 2 | 94 | π*( N^N) |
| | H | -7.40 | 0 | 0 | 100 | π(N^N) |
| **1c** | | | Ir | C^N | N^N | |
| | L | -5.32 | 4 | 1 | 95 | π*( N^N) |
| | H | -7.35 | 0 | 0 | 100 | π(N^N) |
| **2** | | | Ir | C^N | N^N | |
| | L | -4.35 | 2 | 1 | 97 | π*( N^N) |
| | H | -8.02 | 26 | 72 | 2 | d(Ir)+π(C^N) |
| **2a** | | | Ir | C^N | N^N | |
| | L | -4.08 | 2 | 2 | 96 | π*( N^N) |
| | H | -7.78 | 25 | 74 | 1 | d(Ir)+π(C^N) |
| **2b** | | | Ir | C^N | N^N | |
| | L | -5.03 | 4 | 1 | 95 | π*( N^N) |
| | H | -7.88 | 28 | 70 | 2 | d(Ir)+π(C^N) |
| **2c** | | | Ir | C^N | N^N | |
| | L | -5.10 | 4 | 1 | 95 | π*( N^N) |
| | H | -8.08 | 30 | 67 | 3 | d(Ir)+π(C^N) |

**Table S13** The xyz coordinates for the optimized structures for **1** in the $S_0$ and $T_1$ states at PBE0/6-31G* level

| | $S_0$ | | | $T_1$ | | |
|---|---|---|---|---|---|---|
| Ir | -3.36056800 | 0.18187000 | -0.09182900 | -3.35420400 | 0.18088900 | -0.08269400 |
| F | -7.67405900 | -2.56696300 | 1.11376100 | -7.69030000 | -2.60592700 | 1.10335700 |
| F | -4.60874200 | -2.15429800 | 4.59633600 | -4.59669600 | -2.21537000 | 4.57884100 |
| F | 0.73634500 | -3.01545300 | 0.73623300 | 0.73079700 | -3.04659400 | 0.67730800 |
| F | -2.32012100 | -4.57898100 | -2.41146700 | -2.35611800 | -4.54731800 | -2.47115600 |
| N | -1.74517200 | 0.42998100 | 1.15259100 | -1.72199300 | 0.41081300 | 1.15705400 |
| C | -0.83080100 | -0.58169200 | 1.15273900 | -0.81562400 | -0.60712900 | 1.13814700 |
| C | 0.29692200 | -0.49304600 | 1.97834500 | 0.32016900 | -0.53574700 | 1.95405000 |
| H | 1.02197700 | -1.29354500 | 1.97305600 | 1.03939400 | -1.34128500 | 1.93502300 |
| C | 0.47686200 | 0.61490700 | 2.78928900 | 0.51638200 | 0.56400600 | 2.77261400 |
| H | 1.35131500 | 0.67782800 | 3.43025600 | 1.39747800 | 0.61430400 | 3.40556600 |
| C | -0.46862800 | 1.63798100 | 2.77305200 | -0.42016700 | 1.59542900 | 2.77375000 |
| H | -0.36924800 | 2.52108700 | 3.39455000 | -0.30695400 | 2.47245900 | 3.40145600 |
| C | -1.56192400 | 1.50278700 | 1.93739900 | -1.52282800 | 1.47599100 | 1.94764300 |
| H | -2.33375400 | 2.26167100 | 1.88494100 | -2.28984500 | 2.24078000 | 1.90817500 |
| C | -2.36038000 | -1.50759200 | -0.49901500 | -2.36393500 | -1.50465700 | -0.51575500 |
| C | -1.16384100 | -1.67181600 | 0.24768600 | -1.16351600 | -1.68375200 | 0.22138700 |
| C | -0.40427000 | -2.83210300 | 0.05520900 | -0.41306800 | -2.84623800 | 0.00685900 |
| C | -0.76846600 | -3.82477900 | -0.83500700 | -0.79021200 | -3.82347200 | -0.89495000 |
| H | -0.16389000 | -4.71516600 | -0.95888900 | -0.19129600 | -4.71513800 | -1.03636700 |
| C | -1.94451100 | -3.63550200 | -1.54800800 | -1.97010200 | -3.61798500 | -1.59778200 |
| C | -2.73890100 | -2.50596600 | -1.39882600 | -2.75670600 | -2.48623900 | -1.42745700 |
| H | -3.65029600 | -2.43871000 | -1.98344400 | -3.67230900 | -2.40137700 | -2.00287300 |
| N | -4.97363200 | -0.29357200 | -1.27726200 | -4.94751700 | -0.24953500 | -1.26687400 |
| C | -5.94373100 | -1.04558600 | -0.68324300 | -5.95831500 | -1.04661400 | -0.64790600 |
| C | -7.06786100 | -1.43261700 | -1.42443400 | -7.10400200 | -1.43087500 | -1.42760300 |
| H | -7.83241100 | -2.03202800 | -0.95155200 | -7.85683300 | -2.05062700 | -0.96058400 |
| C | -7.18752000 | -1.05496300 | -2.75165600 | -7.23714300 | -1.03147900 | -2.72370900 |
| H | -8.05752700 | -1.36054500 | -3.32516400 | -8.10152000 | -1.32743200 | -3.30825500 |
| C | -6.18380100 | -0.28825200 | -3.33969400 | -6.21714400 | -0.22284100 | -3.30189600 |
| H | -6.23547400 | 0.02502300 | -4.37650600 | -6.27792600 | 0.11954500 | -4.32855800 |
| C | -5.09639900 | 0.06882000 | -2.56372400 | -5.11160800 | 0.12452200 | -2.53160400 |
| H | -4.28071200 | 0.65826200 | -2.96567700 | -4.31268900 | 0.72511600 | -2.95415000 |
| C | -4.42275300 | -0.89080800 | 1.21373100 | -4.40150100 | -0.87209800 | 1.22481100 |
| C | -5.66008000 | -1.37140700 | 0.70689700 | -5.68048600 | -1.36872100 | 0.67538400 |
| C | -6.49620900 | -2.10533800 | 1.55805300 | -6.51812400 | -2.14585100 | 1.56033700 |
| C | -6.16750400 | -2.38172500 | 2.87124400 | -6.16589100 | -2.42549800 | 2.84276200 |
| H | -6.83314900 | -2.95377000 | 3.50621200 | -6.81570800 | -3.01100900 | 3.48325200 |
| C | -4.95060000 | -1.90102800 | 3.33396600 | -4.92763400 | -1.93809200 | 3.32090800 |
| C | -4.08061000 | -1.16665800 | 2.53726800 | -4.06204700 | -1.18222600 | 2.52947500 |
| H | -3.14361500 | -0.83424000 | 2.97053100 | -3.12276300 | -0.85909000 | 2.96569100 |
| N | -4.36481400 | 2.08677700 | 0.33538800 | -4.36268600 | 2.10028700 | 0.36308000 |
| C | -4.07114800 | 3.12187800 | -0.48461300 | -4.07387500 | 3.13384300 | -0.45872900 |
| C | -4.70505700 | 4.35651400 | -0.35849800 | -4.70890800 | 4.36791500 | -0.32981900 |
| H | -4.44879800 | 5.16802000 | -1.03129000 | -4.45587700 | 5.18093500 | -1.00199300 |
| C | -5.66057000 | 4.52751100 | 0.63425400 | -5.66270900 | 4.53583100 | 0.66515300 |
| H | -6.16640700 | 5.48129800 | 0.74919000 | -6.17054500 | 5.48842600 | 0.78136200 |
| C | -5.95652500 | 3.45963200 | 1.47630800 | -5.95471300 | 3.46742900 | 1.50816800 |
| H | -6.69463100 | 3.54862800 | 2.26607400 | -6.69279000 | 3.55458300 | 2.29817900 |
| C | -5.28773900 | 2.25740900 | 1.29112800 | -5.28102700 | 2.26808800 | 1.32185800 |
| H | -5.48087200 | 1.39305500 | 1.91843000 | -5.46357000 | 1.40340100 | 1.95279100 |
| N | -2.49256900 | 1.62835300 | -1.49860300 | -2.49071100 | 1.64613500 | -1.48123600 |
| N | -1.60568100 | 1.62466300 | -2.49918200 | -1.60859600 | 1.64879500 | -2.48609100 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | -1.57597300 | 2.82495400 | -3.12117500 | -1.58870200 | 2.84974200 | -3.10648500 |
| H | -0.90145600 | 3.00226900 | -3.94693600 | -0.91909500 | 3.03201300 | -3.93515200 |
| C | -2.49334200 | 3.64645700 | -2.50249300 | -2.50819300 | 3.66494900 | -2.48263700 |
| H | -2.72697700 | 4.66861200 | -2.76018300 | -2.74940600 | 4.68581400 | -2.73838000 |
| C | -3.04645000 | 2.85121500 | -1.48497500 | -3.05236700 | 2.86546000 | -1.46371600 |
| C | -0.70354400 | 0.50850800 | -2.72558400 | -0.70565500 | 0.53572200 | -2.72281700 |
| H | -0.48323000 | 0.50467800 | -3.79934400 | -0.48672000 | 0.54151700 | -3.79680200 |
| H | -1.25868300 | -0.40618100 | -2.49872300 | -1.25998500 | -0.38145400 | -2.50423500 |
| C | 0.57046900 | 0.57571500 | -1.91264500 | 0.56925700 | 0.59681000 | -1.91100700 |
| C | 1.36381100 | -0.57128000 | -1.83037500 | 1.36438800 | -0.54969300 | -1.83950000 |
| H | 1.03958200 | -1.48997800 | -2.31453600 | 1.04146300 | -1.46437700 | -2.33210100 |
| C | 2.55291700 | -0.55995100 | -1.11511700 | 2.55439700 | -0.54272300 | -1.12561200 |
| H | 3.13609000 | -1.47316800 | -1.03737100 | 3.13898700 | -1.45574700 | -1.05658000 |
| C | 2.99513300 | 0.60078600 | -0.46301000 | 2.99577900 | 0.61304000 | -0.46413600 |
| C | 2.19497000 | 1.74508800 | -0.55634700 | 2.19425700 | 1.75722900 | -0.54762000 |
| H | 2.52577700 | 2.66786500 | -0.08800900 | 2.52471600 | 2.67674500 | -0.07268100 |
| C | 0.99955600 | 1.73429700 | -1.26803900 | 0.99797700 | 1.75075300 | -1.25784300 |
| H | 0.40920700 | 2.64579100 | -1.31987300 | 0.40658700 | 2.66197000 | -1.30231800 |
| C | 4.26201100 | 0.61335000 | 0.29818400 | 4.26274300 | 0.62048600 | 0.29704100 |
| C | 4.38485800 | 1.34860200 | 1.48256800 | 4.38573300 | 1.34835400 | 1.48601500 |
| H | 3.53043000 | 1.90333400 | 1.86285400 | 3.53183300 | 1.90200200 | 1.86903300 |
| C | 5.58286900 | 1.36717600 | 2.18911400 | 5.58334400 | 1.36157800 | 2.19334500 |
| H | 5.65521700 | 1.94658700 | 3.10730600 | 5.65570500 | 1.93544200 | 3.11501700 |
| C | 6.68882200 | 0.64872100 | 1.73638700 | 6.68895000 | 0.64497400 | 1.73684800 |
| C | 6.57268800 | -0.08989200 | 0.55574200 | 6.57287100 | -0.08594600 | 0.55141000 |
| H | 7.43589300 | -0.63810000 | 0.18738400 | 7.43587000 | -0.63245500 | 0.18005900 |
| C | 5.37877900 | -0.10557000 | -0.15135400 | 5.37932900 | -0.09626600 | -0.15644600 |
| H | 5.32043400 | -0.65980900 | -1.08446400 | 5.32130800 | -0.64443500 | -1.09314800 |
| C | 7.98543400 | 0.65277700 | 2.51530900 | 7.98488900 | 0.64286500 | 2.51695200 |
| H | 7.95748100 | 1.41944000 | 3.29617200 | 7.95762500 | 1.40595000 | 3.30133700 |
| H | 8.14544600 | -0.31373000 | 3.00384400 | 8.14236700 | -0.32622000 | 3.00121500 |
| N | 9.77293200 | -0.15115700 | 1.12091000 | 9.77173700 | -0.15818500 | 1.12018600 |
| N | 9.14915500 | 0.88608300 | 1.69065200 | 9.14992400 | 0.87763700 | 1.69470800 |
| C | 9.65903400 | 2.08040000 | 1.29402400 | 9.66339000 | 2.07275200 | 1.30510100 |
| H | 9.25845200 | 3.01380600 | 1.66446100 | 9.26485800 | 3.00520600 | 1.68013100 |
| C | 10.68726200 | 1.80461100 | 0.42526700 | 10.69187900 | 1.79893300 | 0.43605600 |
| H | 11.34507200 | 2.49300100 | -0.08213000 | 11.35205800 | 2.48830800 | -0.06690600 |
| C | 10.71703500 | 0.39449100 | 0.35096000 | 10.71810400 | 0.38914800 | 0.35423300 |
| N | 12.50270100 | 0.23489600 | -1.21455900 | 12.50502800 | 0.23345900 | -1.21020900 |
| C | 11.63956300 | -0.43092800 | -0.43582800 | 11.63949600 | -0.43438200 | -0.43588200 |
| C | 11.60519800 | -1.82834600 | -0.36450000 | 11.60174900 | -1.83205100 | -0.37185200 |
| H | 10.88801400 | -2.31289200 | 0.28982300 | 10.88276000 | -2.31831400 | 0.27921000 |
| C | 12.50140700 | -2.55501000 | -1.13516100 | 12.49704400 | -2.55681400 | -1.14536900 |
| H | 12.50153800 | -3.64131100 | -1.10024600 | 12.49458000 | -3.64327800 | -1.11613200 |
| C | 13.40069800 | -1.87039300 | -1.94831600 | 13.39879800 | -1.87009400 | -1.95400400 |
| H | 14.12094500 | -2.39726200 | -2.56657000 | 14.11844200 | -2.39543000 | -2.57425700 |
| C | 13.35565700 | -0.47881300 | -1.94594500 | 13.35707400 | -0.47843300 | -1.94441100 |
| H | 14.04384700 | 0.09413000 | -2.56590600 | 14.04727700 | 0.09610200 | -2.56064000 |

**Table S14** The xyz coordinates for the optimized structures for **2** in the $S_0$ and $T_1$ states at PBE0/6-31G* level

| | $S_0$ | | | $T_1$ | | |
|---|---|---|---|---|---|---|
| Ir | -1.52191800 | -0.04680800 | -0.19851600 | -1.51670800 | -0.05692500 | -0.18551000 |
| N | -0.18984700 | 1.64486200 | -0.69577500 | -0.17327500 | 1.65550600 | -0.68730800 |
| C | 0.97155900 | 1.33597000 | -1.31712900 | 0.97221500 | 1.34701600 | -1.33473100 |
| C | 1.88674100 | 2.31345000 | -1.69779500 | 1.87763000 | 2.32574100 | -1.73630500 |
| H | 2.82355800 | 2.03544000 | -2.16960000 | 2.80374400 | 2.04935500 | -2.22963000 |
| C | 1.58853300 | 3.64600300 | -1.44402400 | 1.58190600 | 3.65785000 | -1.47744800 |
| H | 2.29409700 | 4.42345500 | -1.71889100 | 2.27844500 | 4.43683700 | -1.77043100 |
| C | 0.38491000 | 3.96151100 | -0.82174400 | 0.39351200 | 3.97228300 | -0.82583600 |
| H | 0.11115700 | 4.98898800 | -0.60744900 | 0.12313200 | 4.99971600 | -0.60712700 |
| C | -0.47392200 | 2.93157500 | -0.46146800 | -0.45289700 | 2.94002100 | -0.44338100 |
| H | -1.41882800 | 3.12104400 | 0.03751300 | -1.38246000 | 3.12582800 | 0.08561700 |
| N | 1.78474100 | -2.13025700 | -1.85042500 | 1.79483300 | -2.11733100 | -1.87003500 |
| N | 0.55227000 | -2.18246500 | -1.35280800 | 0.57292100 | -2.17612900 | -1.34909100 |
| N | 0.18416900 | -0.95375900 | -1.16093000 | 0.19904800 | -0.94917000 | -1.15752400 |
| C | 1.17609300 | -0.09000800 | -1.52418600 | 1.17677700 | -0.07946300 | -1.54344000 |
| C | 2.22140500 | -0.85940600 | -1.98261900 | 2.21905700 | -0.84392400 | -2.01716300 |
| H | 3.21136500 | -0.62015400 | -2.33886400 | 3.19992200 | -0.59954600 | -2.39445500 |
| C | 2.50371300 | -3.37005000 | -2.13236200 | 2.51950300 | -3.35249400 | -2.15711800 |
| H | 2.48880600 | -3.54770400 | -3.21260200 | 2.50609300 | -3.52478200 | -3.23819600 |
| H | 1.91174300 | -4.15717900 | -1.65524000 | 1.93049900 | -4.14435700 | -1.68423900 |
| N | 5.34019800 | 3.15066800 | -0.42150300 | 5.32827200 | 3.18337600 | -0.36595000 |
| C | 4.65561700 | 2.83305500 | 0.68697800 | 4.62123200 | 2.84328700 | 0.72144900 |
| C | 3.94583000 | 3.77253900 | 1.44168300 | 3.88088100 | 3.76400900 | 1.46971700 |
| H | 3.41735400 | 3.45515900 | 2.33463400 | 3.33626800 | 3.42938400 | 2.34655300 |
| C | 3.96261100 | 5.09939000 | 1.03153700 | 3.88834800 | 5.09556800 | 1.07478700 |
| H | 3.43619500 | 5.85816000 | 1.60425400 | 3.33780700 | 5.84029900 | 1.64325300 |
| C | 4.68050100 | 5.44262900 | -0.11169100 | 4.62808600 | 5.46190000 | -0.04699600 |
| H | 4.73569300 | 6.46978700 | -0.45897200 | 4.67659800 | 6.49360500 | -0.38156900 |
| C | 5.34810600 | 4.42916900 | -0.79713900 | 5.32700900 | 4.46596700 | -0.72696200 |
| H | 5.92354200 | 4.65747600 | -1.69293100 | 5.92094300 | 4.71271900 | -1.60562900 |
| N | 5.24718700 | -0.62997400 | 1.41436900 | 5.23911400 | -0.62216200 | 1.41464900 |
| N | 4.16505400 | -0.37583500 | 2.16498300 | 4.14174500 | -0.38992700 | 2.14985100 |
| N | 3.84151000 | 0.86598900 | 1.97942900 | 3.80758000 | 0.85085200 | 1.97504100 |
| C | 4.70970100 | 1.42820900 | 1.09431700 | 4.68435200 | 1.43420800 | 1.11248900 |
| C | 5.61843200 | 0.46159600 | 0.71607000 | 5.61005300 | 0.48259600 | 0.73736200 |
| H | 6.46507300 | 0.48780500 | 0.04798000 | 6.46706300 | 0.52682300 | 0.08361100 |
| C | 5.81027900 | -1.96999100 | 1.38694200 | 5.81411800 | -1.95669400 | 1.37544800 |
| H | 5.35611400 | -2.49215800 | 2.23430200 | 5.36603800 | -2.49040100 | 2.21886800 |
| H | 6.88692900 | -1.90348900 | 1.56909400 | 6.89023700 | -1.88144300 | 1.55696400 |
| C | 3.92092800 | -3.32644000 | -1.61512800 | 3.93593300 | -3.30478600 | -1.63781100 |
| C | 4.21075600 | -2.73928100 | -0.38449200 | 4.22105500 | -2.72020700 | -0.40489900 |
| H | 3.41621300 | -2.30343400 | 0.21868600 | 3.42374200 | -2.28866700 | 0.19768300 |
| C | 5.52352100 | -2.67342100 | 0.08161900 | 5.53239400 | -2.65277900 | 0.06492500 |
| C | 6.54797800 | -3.24063000 | -0.67502700 | 6.56033300 | -3.21423300 | -0.69130400 |
| H | 7.57448900 | -3.19524200 | -0.31942500 | 7.58583500 | -3.16735700 | -0.33299000 |
| C | 6.26119900 | -3.85657500 | -1.89077200 | 6.27832800 | -3.82657000 | -1.90997300 |
| H | 7.06203100 | -4.29433400 | -2.47899500 | 7.08193900 | -4.25963600 | -2.49787700 |
| C | 4.95527800 | -3.88475000 | -2.36895500 | 4.97355900 | -3.85754600 | -2.39115600 |
| H | 4.74112600 | -4.34111900 | -3.33247400 | 4.76295900 | -4.31172800 | -3.35648900 |
| N | -0.64493500 | -0.56215800 | 1.59021900 | -0.64174700 | -0.59477500 | 1.60737400 |
| C | -1.16474900 | -1.66218600 | 2.20775500 | -1.17127300 | -1.69754800 | 2.21021100 |
| C | -0.63713300 | -2.07362300 | 3.43843700 | -0.65112200 | -2.12791800 | 3.43720700 |
| H | -1.05962300 | -2.93749200 | 3.93098500 | -1.08201200 | -2.99340400 | 3.91953600 |

| | | | | | | |
|---|---|---|---|---|---|---|
| C | 0.41865700 | -1.38084600 | 4.00814800 | 0.41063600 | -1.45119300 | 4.01577800 |
| H | 0.82770600 | -1.70586700 | 4.96029900 | 0.81452700 | -1.79020200 | 4.96526600 |
| C | 0.95362600 | -0.27799900 | 3.34735900 | 0.95871900 | -0.34768400 | 3.36716700 |
| H | 1.80241800 | 0.27724500 | 3.72821000 | 1.81259000 | 0.19454700 | 3.75526100 |
| C | 0.38537300 | 0.09663800 | 2.14381100 | 0.39548600 | 0.04668500 | 2.16713300 |
| H | 0.76184600 | 0.94853200 | 1.59068200 | 0.78207200 | 0.90014100 | 1.62306700 |
| C | -2.58690100 | -1.68468500 | 0.23315900 | -2.58109800 | -1.69629600 | 0.22290800 |
| C | -2.24185300 | -2.29859600 | 1.46515700 | -2.24678300 | -2.32092600 | 1.45277700 |
| C | -2.92913400 | -3.45461300 | 1.85495500 | -2.94301000 | -3.47713600 | 1.82516900 |
| C | -3.92885800 | -4.02300800 | 1.08987900 | -3.93671800 | -4.03466100 | 1.04406500 |
| H | -4.44495200 | -4.91708400 | 1.41777500 | -4.45838000 | -4.93041900 | 1.35851500 |
| C | -4.24142300 | -3.39617000 | -0.10800000 | -4.23586000 | -3.39752600 | -0.15223600 |
| C | -3.59744800 | -2.24694100 | -0.54508200 | -3.58434800 | -2.24665300 | -0.57289800 |
| H | -3.90727200 | -1.81409000 | -1.48988600 | -3.88000400 | -1.80116800 | -1.51602800 |
| F | -2.62727500 | -4.06360400 | 3.01279800 | -2.65623200 | -4.09704700 | 2.98064000 |
| F | -5.20389400 | -3.92427100 | -0.86621200 | -5.19174100 | -3.91698900 | -0.92340800 |
| N | -2.59810600 | 0.40059000 | -1.88930600 | -2.54330900 | 0.39472400 | -1.87495200 |
| C | -3.69687300 | 1.18690400 | -1.70576100 | -3.69127800 | 1.22103100 | -1.68163500 |
| C | -4.49435300 | 1.52524000 | -2.80708100 | -4.48887200 | 1.56620800 | -2.82531200 |
| H | -5.36592300 | 2.14635400 | -2.65804000 | -5.36396500 | 2.18280900 | -2.67266600 |
| C | -4.17033100 | 1.05431300 | -4.06859300 | -4.15993400 | 1.12088800 | -4.07083100 |
| H | -4.79377000 | 1.31264700 | -4.91941000 | -4.76890200 | 1.38012900 | -4.93015600 |
| C | -3.04891400 | 0.24353900 | -4.23161600 | -3.00734500 | 0.29674100 | -4.22489200 |
| H | -2.76637700 | -0.15505900 | -5.19963600 | -2.71194600 | -0.08985600 | -5.19354300 |
| C | -2.29309800 | -0.05708300 | -3.11335700 | -2.25481800 | -0.02858500 | -3.10252100 |
| H | -1.41918500 | -0.69584300 | -3.17104600 | -1.38573100 | -0.67339800 | -3.18696100 |
| C | -2.97636100 | 1.05298500 | 0.61674700 | -2.93858500 | 1.04632000 | 0.63513500 |
| C | -3.91174900 | 1.57361600 | -0.31887400 | -3.90173800 | 1.57699000 | -0.35277600 |
| C | -4.94827400 | 2.39191000 | 0.14806200 | -4.96921100 | 2.40607800 | 0.15143200 |
| C | -5.09944000 | 2.71519700 | 1.48254700 | -5.10600400 | 2.69788100 | 1.47198700 |
| H | -5.91259400 | 3.34811800 | 1.81665100 | -5.91954300 | 3.32348700 | 1.82150700 |
| C | -4.17148800 | 2.18837900 | 2.37093800 | -4.16562900 | 2.16050000 | 2.38268700 |
| C | -3.12271600 | 1.37279600 | 1.96681600 | -3.10877000 | 1.35077700 | 1.97630300 |
| H | -2.44285200 | 0.99416600 | 2.72226000 | -2.43611100 | 0.96439300 | 2.73464300 |
| F | -5.84352400 | 2.90470200 | -0.70998600 | -5.86031000 | 2.91417900 | -0.71211900 |
| F | -4.29665100 | 2.48590300 | 3.66428300 | -4.31351300 | 2.46101200 | 3.67115900 |