

## **The effect of anion complexation on the aromatic properties of aromatic and antiaromatic porphyrinoids**

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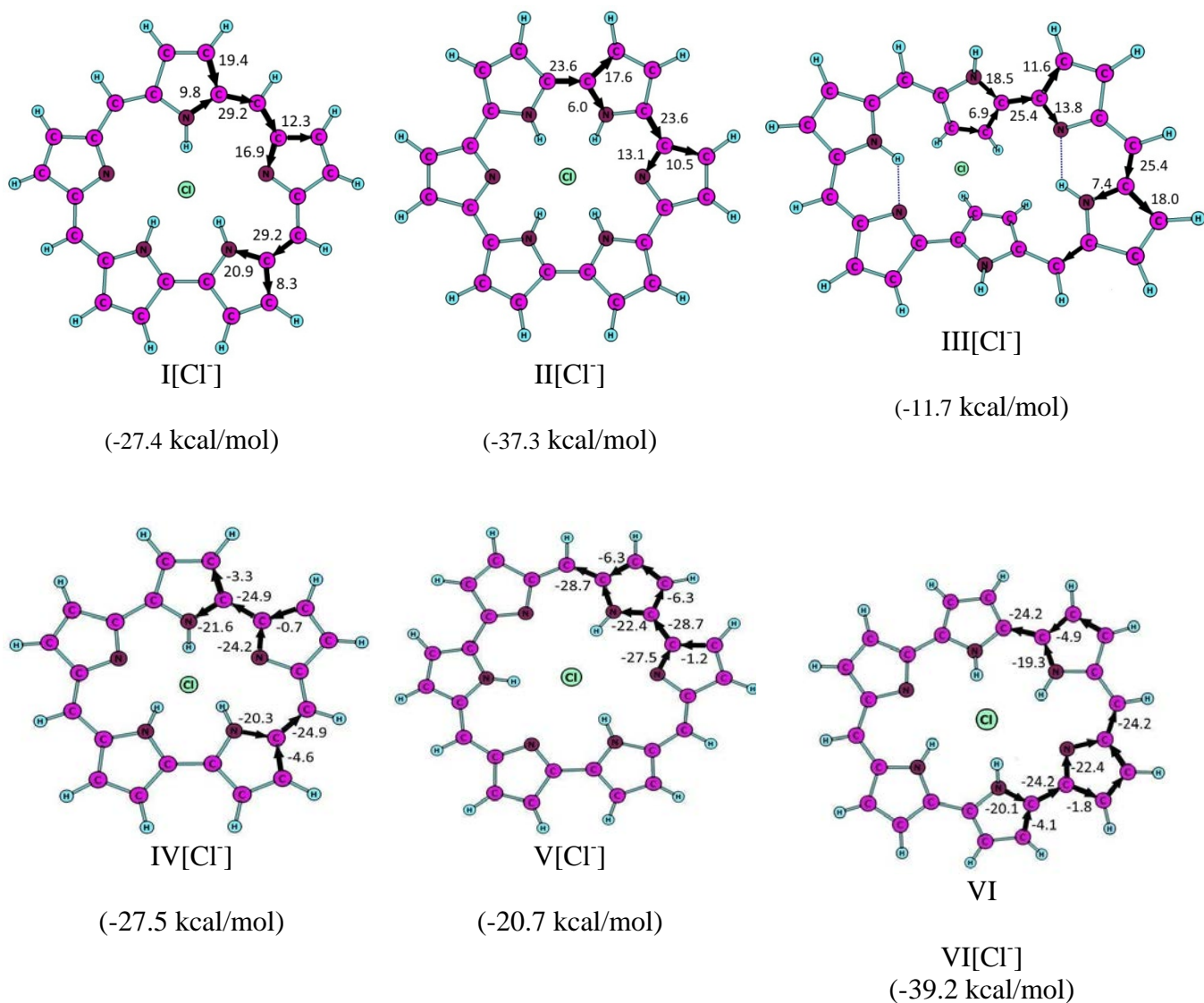
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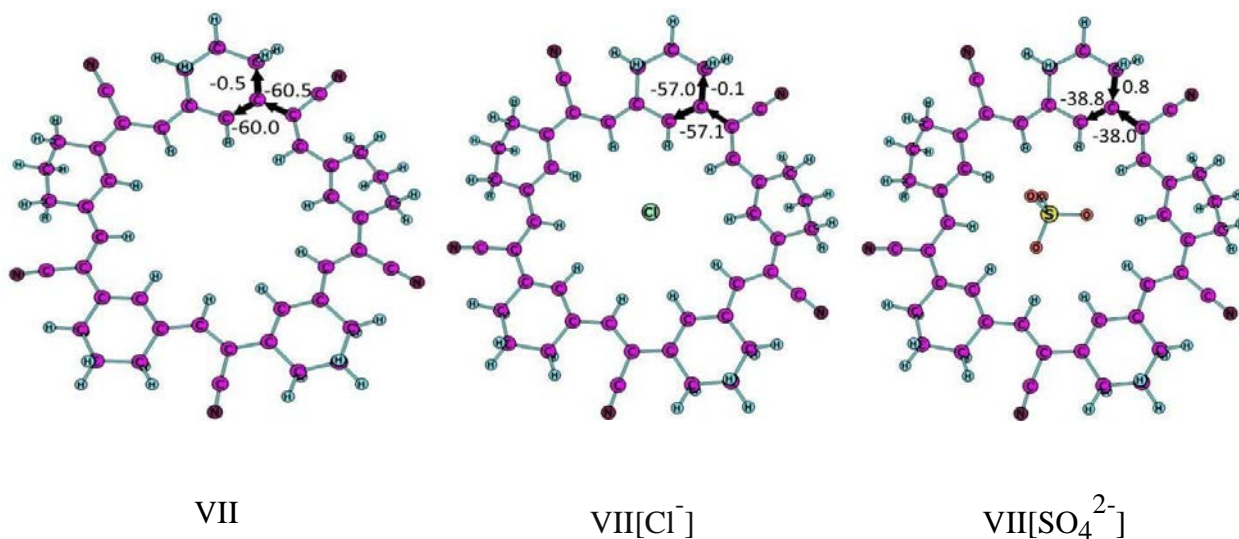
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## Ring-current strengths and pathways

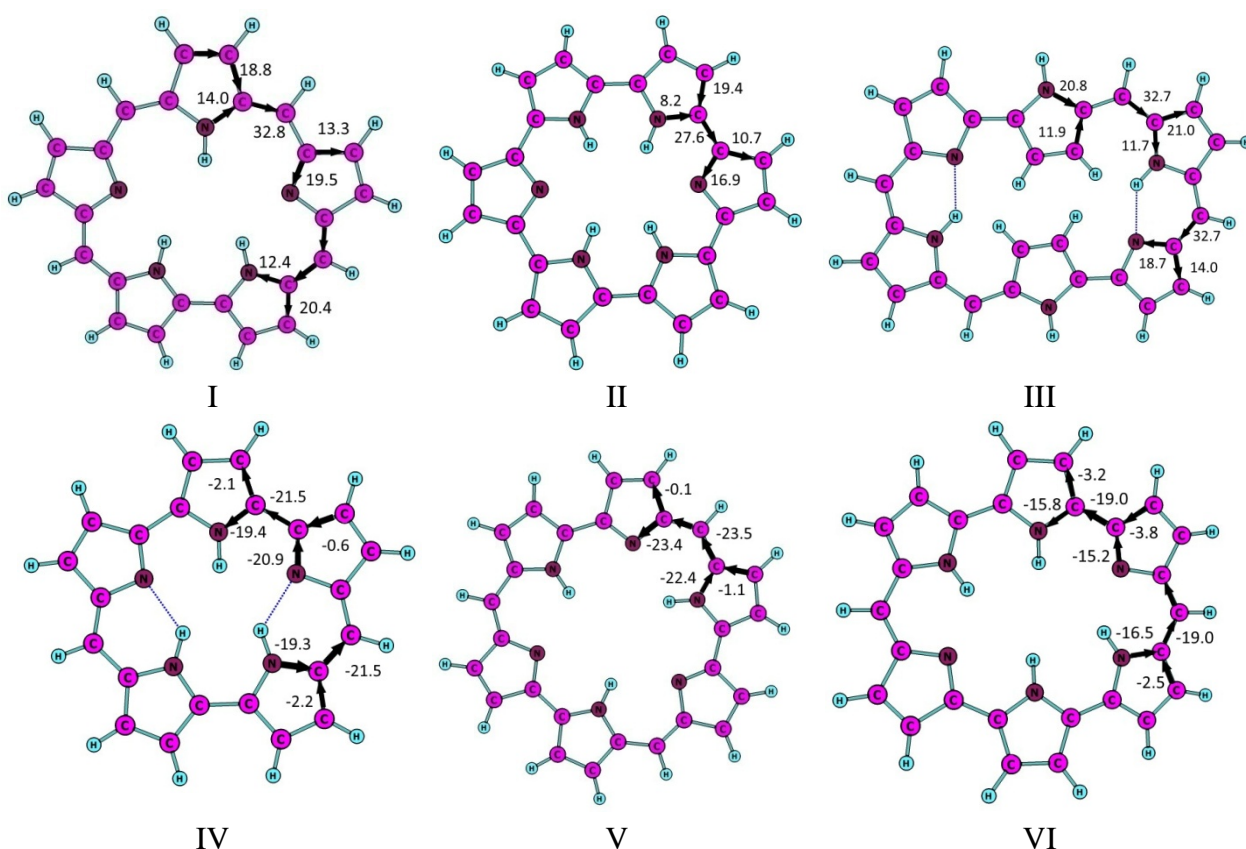


**Figure S1.** The molecular structures of I[Cl<sup>-</sup>], II[Cl<sup>-</sup>], III[Cl<sup>-</sup>], IV[Cl<sup>-</sup>], V[Cl<sup>-</sup>], and VI[Cl<sup>-</sup>].

Integrated current strength susceptibilities (in nA/T) calculated at the B3LYP/def2-TZVP level are also given. The current pathways are shown with black arrows. BSSE-corrected binding energies (in kcal/mol) of the Cl<sup>-</sup> complexes calculated at the B3LYP/def2-TZVP level are also reported.



**Figure S2.** The molecular structures of VII, VII[Cl<sup>-</sup>], and VII[SO<sub>4</sub><sup>2-</sup>]. Integrated current strength susceptibilities (in nA/T) calculated at the B3LYP/def2-TZVP level are also given. The current pathways are shown with black arrows.



**Figure S3.** The molecular structures of the studied porphyrinoids. Current strengths (in nA/T) along different pathways calculated at the M06-2X/def2-TZVP level are also given. The current pathways are shown with black arrows.

**Table S1.** Ring-current strengths (in nA/T) of I, II, III, I[Cl<sup>-</sup>], II[Cl<sup>-</sup>] and III[Cl<sup>-</sup>] calculated at the B3LYP/def2-TZVP level of theory.

| B3LYP    |              |  |
|----------|--------------|--|
| Molecule | Porphyrinoid | The Cl <sup>-</sup> complex <sup>-</sup> |
| I        | 28.2         | 29.2                                     |
| II       | 23.5         | 23.6                                     |
| III      | 28.9         | 25.4                                     |

**Table S2.** Ring-current strengths (in nA/T) of IV, V, VI, IV[Cl<sup>-</sup>], V[Cl<sup>-</sup>] and VI[Cl<sup>-</sup>] calculated at the B3LYP/def2-TZVP level of theory.

| B3LYP    |              |  |
|----------|--------------|--|
| Molecule | Porphyrinoid | The Cl <sup>-</sup> complex <sup>-</sup> |
| IV       | -36.1        | -24.9                                    |
| V        | -39.7        | -28.7                                    |
| VI       | -30.9        | -24.2                                    |

**Table S3.** Ring-current strengths (nA/T) of molecule VII, VII[Cl<sup>-</sup>], and VII[SO<sub>4</sub><sup>2-</sup>] calculated at B3LYP/def2-TZVP level of theory.

| Molecule                            | Ring-current strengths (nA/T) |
|-------------------------------------|-------------------------------|
| VII                                 | -60.5                         |
| VII[Cl <sup>-</sup> ]               | -57.1                         |
| VII[SO <sub>4</sub> <sup>2-</sup> ] | -38.0                         |

**Table S4.** Vertical excitation energies (in eV) of the I[Cl<sup>-</sup>], II[Cl<sup>-</sup>] and III[Cl<sup>-</sup>] complexes calculated at the B3LYP and M06-2X levels. The oscillator strength and absorption wave length ( $\lambda$  in nm) are also given. The main orbital character of the transition is reported.

| B3LYP    |                 |             |            |        |                |
|----------|-----------------|-------------|------------|--------|----------------|
| Molecule | ExcitedState    | Coefficient | Energy(eV) | f      | $\lambda$ (nm) |
| I        | 1 HOMO-1→LUMO   | 0.46        | 1.94       | 0.0004 | 637            |
|          | HOMO→LUMO+1     | 0.53        |            |        |                |
|          | 2 HOMO-1→LUMO+1 | -0.40       | 2.01       | 0.03   | 617            |
|          | HOMO→LUMO       | 0.58        |            |        |                |
|          | 3 HOMO-2→LUMO   | 0.69        | 2.24       | 0.003  | 552            |
|          | HOMO-1→LUMO     | -0.11       |            |        |                |
|          | 4 HOMO-3→LUMO   | 0.54        | 2.41       | 0.005  | 513            |
|          | HOMO-2→LUMO+1   | -0.42       |            |        |                |
| II       | HOMO-1→LUMO+1   | 0.16        |            |        |                |
|          | 1 HOMO-2→LUMO   | 0.15        | 1.75       | 0.24   | 710            |
|          | HOMO-1→LUMO     | 0.67        |            |        |                |
|          | HOMO→LUMO+1     | 0.17        |            |        |                |
|          | 2 HOMO-1→LUMO+1 | -0.18       | 1.85       | 0.4    | 670            |

|               |   | HOMO→LUMO     | 0.70        |            |        |       |
|---------------|---|---------------|-------------|------------|--------|-------|
|               | 3 | HOMO-2→LUMO   | 0.69        | 2          | 0.03   | 618   |
|               |   | HOMO-1→LUMO   | -0.14       |            |        |       |
|               | 4 | HOMO-3→LUMO   | 0.71        | 2.3        | 0      | 545   |
|               | 1 | HOMO→LUMO     | 0.70        | 0.52       | 0.0004 | 2394  |
|               | 2 | HOMO-1→LUMO   | 0.70        | 0.54       | 0      | 2307  |
| III           | 3 | HOMO-2→LUMO   | 0.71        | 0.58       | 0.0002 | 2124  |
|               | 4 | HOMO-1→LUMO+1 | 0.34        | 1.1        | 0.0015 | 1124  |
|               |   | HOMO→LUMO+1   | 0.62        |            |        |       |
| <b>M06-2X</b> |   |               |             |            |        |       |
| Molecule      |   | ExcitedState  | Coefficient | Energy(eV) | f      | λ(nm) |
|               | 1 | HOMO-1→LUMO+1 | -0.42       | 2.12       | 0.02   | 585   |
|               |   | HOMO→LUMO     | 0.56        |            |        |       |
|               | 2 | HOMO-1→LUMO   | 0.51        | 2.17       | 0.014  | 572   |
|               |   | HOMO→LUMO+1   | 0.49        |            |        |       |
| I             | 3 | HOMO-2→LUMO   | -0.35       | 3.14       | 0.825  | 395   |
|               |   | HOMO-1→LUMO   | -0.43       |            |        |       |
|               |   | HOMO→LUMO+1   | 0.44        |            |        |       |
|               | 4 | HOMO-2→LUMO   | 0.60        | 3.19       | 0.3    | 388   |
|               |   | HOMO-1→LUMO   | -0.24       |            |        |       |
|               |   | HOMO→LUMO+1   | 0.25        |            |        |       |
|               | 1 | HOMO-1→LUMO   | 0.68        | 1.73       | 0.35   | 718   |
|               |   | HOMO-1→LUMO+1 | -0.18       |            |        |       |
| II            | 2 | HOMO-1→LUMO+1 | 0.16        | 1.78       | 0.516  | 695   |
|               |   | HOMO→LUMO     | 0.70        |            |        |       |
|               | 3 | HOMO-2→LUMO   | 0.70        | 2.77       | 0.004  | 447   |
|               | 4 | HOMO-5→LUMO   | 0.70        | 2.95       | 0      | 420   |
|               | 1 | HOMO-4→LUMO+1 | 0.20        | 1.67       | 0.064  | 741   |
|               |   | HOMO-3→LUMO   | 0.14        |            |        |       |
|               |   | HOMO-1→LUMO   | 0.20        |            |        |       |
|               |   | HOMO→LUMO     | 0.62        |            |        |       |
|               | 2 | HOMO-4→LUMO+1 | -0.16       | 1.74       | 0.0354 | 714   |
|               |   | HOMO-1→LUMO   | 0.66        |            |        |       |
|               |   | HOMO→LUMO     | -0.16       |            |        |       |
| III           | 3 | HOMO-4→LUMO   | -0.13       | 1.75       | 0.0022 | 708   |
|               |   | HOMO-3→LUMO   | 0.18        |            |        |       |
|               |   | HOMO-2→LUMO   | 0.66        |            |        |       |
|               |   | HOMO→LUMO+1   | 0.11        |            |        |       |
|               | 4 | HOMO-4→LUMO+1 | -0.11       | 1.77       | 0.016  | 701   |
|               |   | HOMO-3→LUMO   | 0.66        |            |        |       |
|               |   | HOMO-2→LUMO   | -0.17       |            |        |       |
|               |   | HOMO→LUMO     | -0.11       |            |        |       |

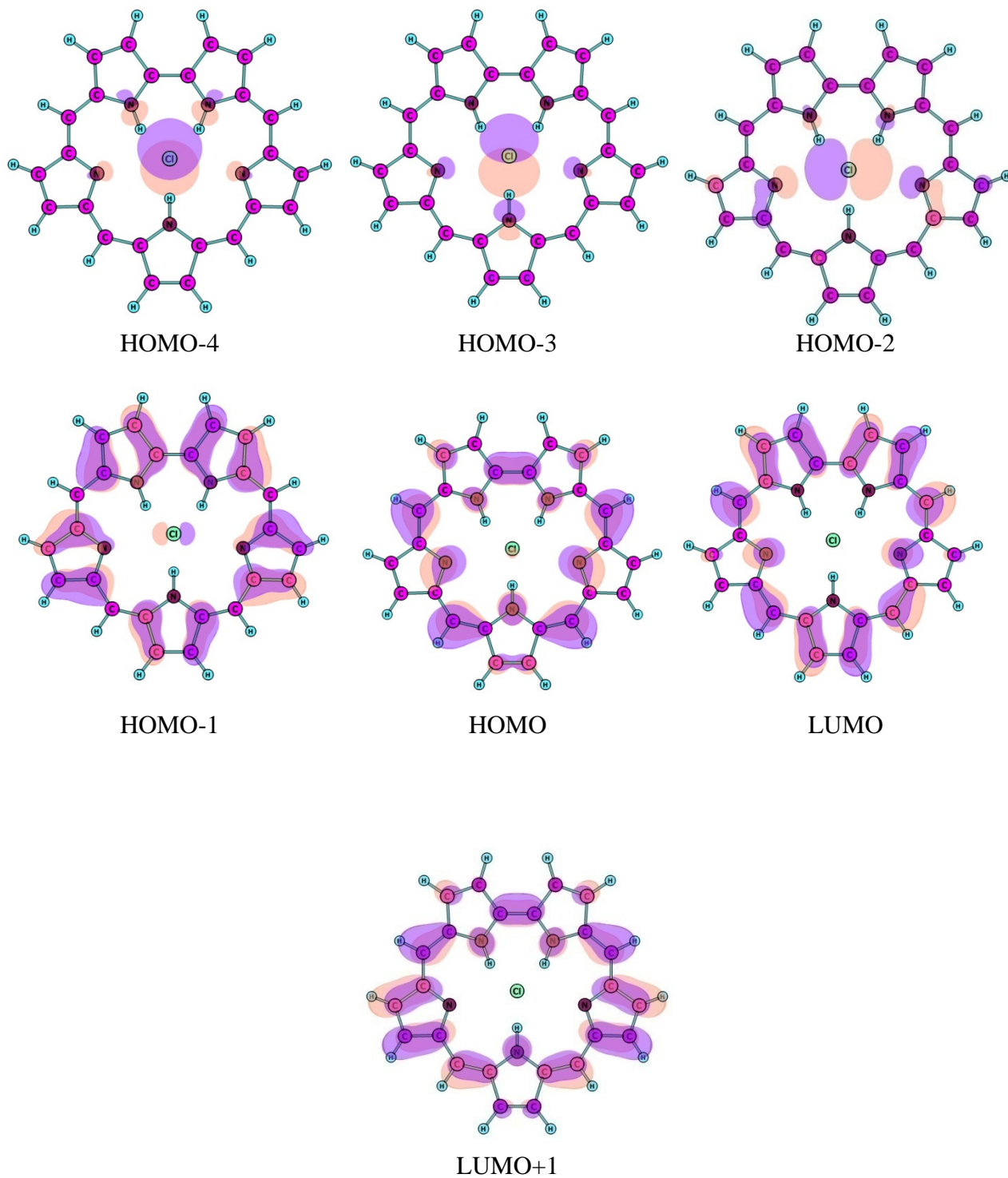
**TableS5.** Vertical excitation energies (in eV) of the IV[Cl<sup>-</sup>], V[Cl<sup>-</sup>] and VI[Cl<sup>-</sup>] complexes calculated at the B3LYP and M06-2X levels. The oscillator strength and absorption wave length ( $\lambda$  in nm) are also given. The main orbital character of the transition is reported.

| <b>B3LYP</b> |              |               |             |            |        |                |
|--------------|--------------|---------------|-------------|------------|--------|----------------|
| Molecule     |              | Excited State | Coefficient | Energy(eV) | f      | $\lambda$ (nm) |
| IV           | 1            | HOMO→LUMO     | 0.71        | 1.12       | 0.004  | 1109           |
|              | 2            | HOMO-1 →LUMO  | 0.71        | 1.76       | 0.0006 | 704            |
|              | 3            | HOMO-2 →LUMO  | 0.71        | 1.84       | 0.00   | 673            |
|              | 4            | HOMO-3→LUMO   | 0.71        | 2.11       | 0.004  | 588            |
| V            | 1            | HOMO→LUMO     | 0.71        | 1.05       | 0.00   | 1179           |
|              | 2            | HOMO-1 →LUMO  | 0.71        | 1.33       | 0.00   | 931            |
|              | 3            | HOMO-2 →LUMO  | 0.71        | 1.36       | 0.0001 | 914            |
|              | 4            | HOMO-3→LUMO   | 0.71        | 1.36       | 0.0001 | 913            |
| VI           | 1            | HOMO→LUMO     | 0.71        | 1.11       | 0.00   | 1116           |
|              | 2            | HOMO-3 →LUMO  | -0.16       | 2.23       | 0.14   | 555            |
|              |              | HOMO-2 →LUMO  | 0.19        |            |        |                |
|              |              | HOMO-1 →LUMO  | -0.21       |            |        |                |
|              |              | HOMO→LUMO+1   | 0.62        |            |        |                |
|              | 3            | HOMO-3 →LUMO  | 0.21        | 2.38       | 0.02   | 521            |
|              |              | HOMO-2 →LUMO  | 0.49        |            |        |                |
|              |              | HOMO-1 →LUMO  | 0.46        |            |        |                |
|              | 4            | HOMO-4 →LUMO  | 0.66        | 2.66       | 0.003  | 466            |
|              |              | HOMO-3 →LUMO  | -0.21       |            |        |                |
|              |              | HOMO-2 →LUMO  | 0.10        |            |        |                |
|              | <b>M062X</b> |               |             |            |        |                |
| Molecule     |              | Excited State | Coefficient | Energy(eV) | f      | $\lambda$ (nm) |
| IV           | 1            | HOMO→LUMO     | 0.70        | 1.60       | 0.001  | 775            |
|              | 2            | HOMO-1 →LUMO  | 0.70        | 2.85       | 0.009  | 435            |
|              | 3            | HOMO-2 →LUMO  | 0.69        | 2.96       | 0.02   | 418            |
|              |              | HOMO→LUMO+1   | -0.14       |            |        |                |
|              | 4            | HOMO-3→LUMO   | 0.44        | 3.13       | 0.33   | 396            |
|              |              | HOMO→LUMO+1   | 0.53        |            |        |                |
| V            | 1            | HOMO→LUMO     | 0.69        | 1.55       | 0.0001 | 798            |
|              | 2            | HOMO-1 →LUMO  | 0.69        | 2.47       | 0.003  | 501            |
|              | 3            | HOMO-3 →LUMO  | 0.62        | 2.48       | 0.003  | 500            |
|              |              | HOMO-2→LUMO   | 0.32        |            |        |                |
|              | 4            | HOMO-3 →LUMO  | -0.31       | 2.52       | 0.0001 | 492            |
|              |              | HOMO-2→LUMO   | 0.62        |            |        |                |
| VI           | 1            | HOMO→LUMO     | 0.69        | 1.63       | 0.00   | 760            |
|              | 2            | HOMO→LUMO+1   | 0.70        | 2.97       | 0.75   | 417            |
|              | 3            | HOMO-6→LUMO+1 | -0.13       | 3.27       | 0.48   | 379            |
|              |              | HOMO-3→LUMO   | -0.11       |            |        |                |
|              |              | HOMO-1→LUMO   | 0.67        |            |        |                |
|              | 4            | HOMO-4→LUMO   | -0.11       | 3.61       | 0.25   | 343            |
|              | HOMO-3→LUMO  | -0.43         |             |            |        |                |

|  |             |       |
|--|-------------|-------|
|  | HOMO-2→LUMO | 0.50  |
|  | HOMO-1→LUMO | -0.15 |

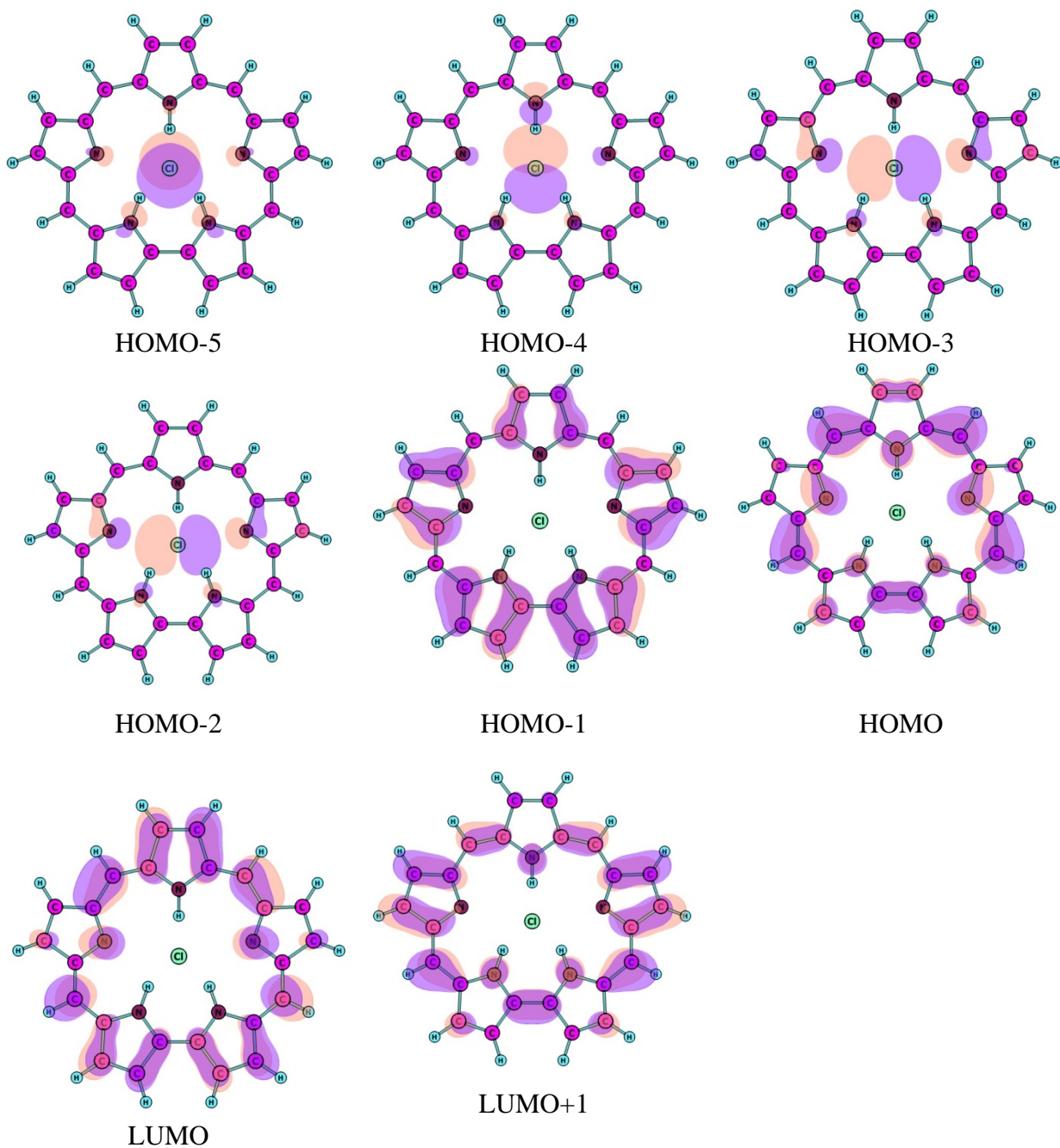
**Table S6.** Vertical excitation energies (in eV) of the VII[Cl<sup>-</sup>] and VII[SO<sub>4</sub><sup>2-</sup>] complexes calculated at the B3LYP and M06-2X levels. The oscillator strength and absorption wave length ( $\lambda$  in nm) are also given. The main orbital character of the transition is reported.

| <b>B3LYP</b>                        |                                     |               |               |             |            |                |                |
|-------------------------------------|-------------------------------------|---------------|---------------|-------------|------------|----------------|----------------|
| Molecule                            |                                     | Excited State | Coefficient   | Energy(eV)  | f          | $\lambda$ (nm) |                |
| VII[Cl <sup>-</sup> ]               | 1                                   | HOMO-2→LUMO   | 0.15          | 0.34        | 0.00       | 3693           |                |
|                                     |                                     | HOMO→LUMO     | 0.69          |             |            |                |                |
|                                     | 2                                   | HOMO-3→LUMO   | -0.12         | 0.47        | 0.0005     | 2657           |                |
|                                     |                                     | HOMO-2→LUMO   | 0.63          |             |            |                |                |
|                                     |                                     | HOMO-1 →LUMO  | -0.24         |             |            |                |                |
|                                     | 3                                   | HOMO→LUMO     | -0.15         |             |            |                |                |
|                                     |                                     | HOMO-3→LUMO   | 0.70          | 0.49        | 0.0001     | 2506           |                |
|                                     | 4                                   | HOMO-2→LUMO   | 0.25          | 0.51        | 0.01       | 2422           |                |
|                                     |                                     | HOMO-1→LUMO   | 0.66          |             |            |                |                |
|                                     | VII[SO <sub>4</sub> <sup>2-</sup> ] | 1             | HOMO-1→LUMO   | 0.72        | 0.24       | 0.00           | 5269           |
|                                     |                                     |               | HOMO-1→LUMO   | -0.14       |            |                |                |
|                                     |                                     | 2             | HOMO-2 →LUMO  | 0.70        | 0.31       | 0.0001         | 4028           |
| HOMO →LUMO                          |                                     |               | 0.10          |             |            |                |                |
| 3                                   |                                     | HOMO-3 →LUMO  | 0.63          | 0.56        | 0.006      | 2218           |                |
|                                     |                                     | HOMO →LUMO    | -0.36         |             |            |                |                |
|                                     |                                     | HOMO→LUMO     | 0.16          |             |            |                |                |
| 4                                   |                                     | HOMO-3 →LUMO  | 0.32          | 0.63        | 0.0006     | 1974           |                |
|                                     |                                     | HOMO →LUMO    | 0.73          |             |            |                |                |
|                                     |                                     |               | HOMO→LUMO     | -0.37       |            |                |                |
| <b>M062X</b>                        |                                     |               |               |             |            |                |                |
| Molecule                            |                                     |               | Excited State | Coefficient | Energy(eV) | f              | $\lambda$ (nm) |
| VII[Cl <sup>-</sup> ]               | 1                                   | HOMO→LUMO     | 0.69          | 0.78        | 0.04       | 1581           |                |
|                                     | 2                                   | HOMO-1 →LUMO  | 0.70          | 1.18        | 0.0001     | 1050           |                |
|                                     | 3                                   | HOMO-2→LUMO   | 0.70          | 1.26        | 0.00       | 987            |                |
|                                     | 4                                   | HOMO-3 →LUMO  | 0.71          | 1.29        | 0.0001     | 958            |                |
| VII[SO <sub>4</sub> <sup>2-</sup> ] | 1                                   | HOMO-3→LUMO   | 0.11          | 0.66        | 0.002      | 1890           |                |
|                                     |                                     | HOMO-2→LUMO   | 0.17          |             |            |                |                |
|                                     |                                     | HOMO →LUMO    | 0.67          |             |            |                |                |
|                                     | 2                                   | HOMO-2→LUMO   | 0.51          | 0.67        | 0.0003     | 1840           |                |
|                                     |                                     | HOMO-1 →LUMO  | -0.46         |             |            |                |                |
|                                     |                                     | HOMO →LUMO    | -0.17         |             |            |                |                |
|                                     | 3                                   | HOMO-2→LUMO   | 0.45          | 0.83        | 0.04       | 1489           |                |
|                                     |                                     | HOMO-1 →LUMO  | 0.52          |             |            |                |                |
|                                     | 4                                   | HOMO-3→LUMO   | 0.70          | 0.87        | 0.0006     | 1423           |                |

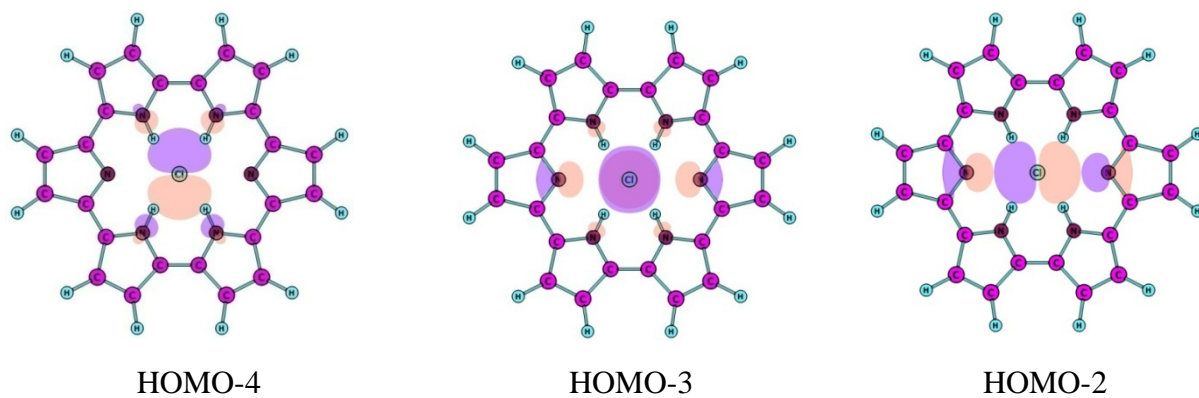


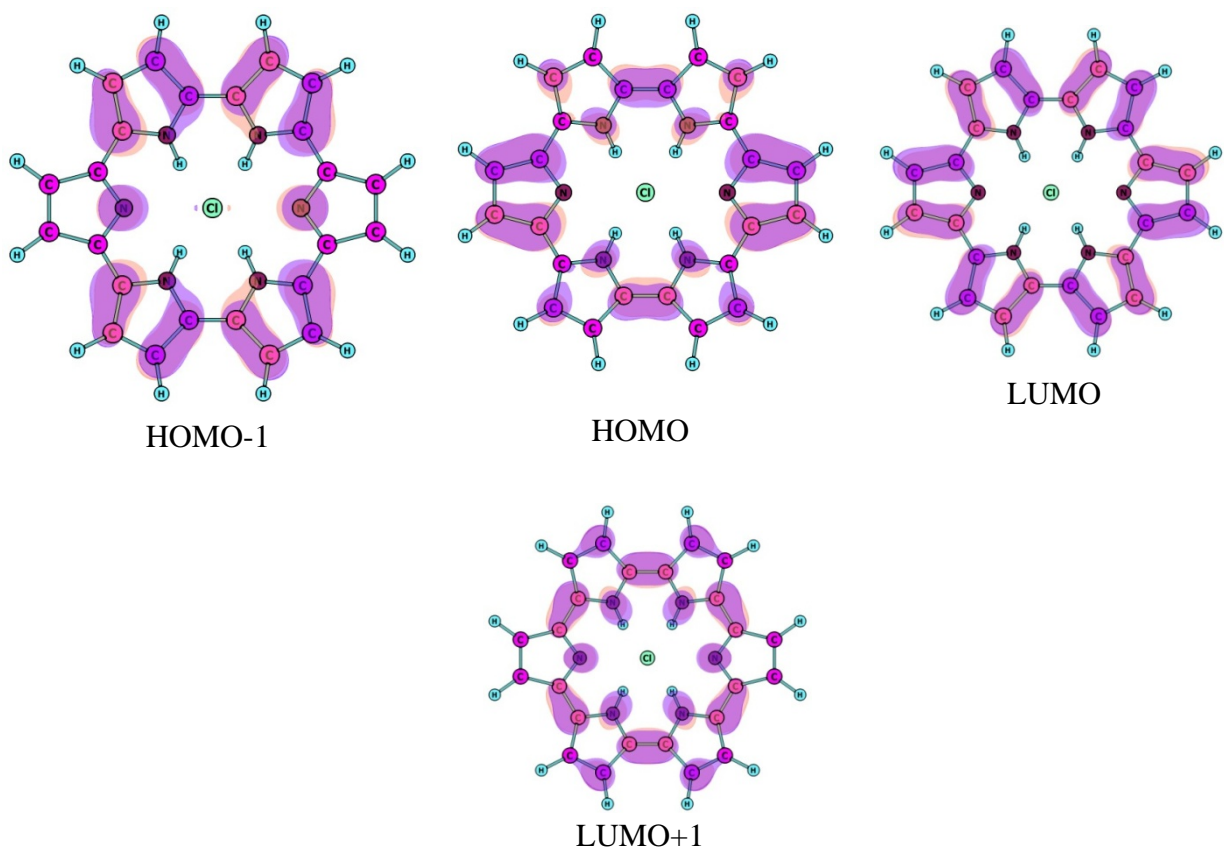
**Figure S4.** Schematic description of frontier orbitals of the  $I[Cl^-]$  complex calculated at the B3LYP/def2-TZVP level.



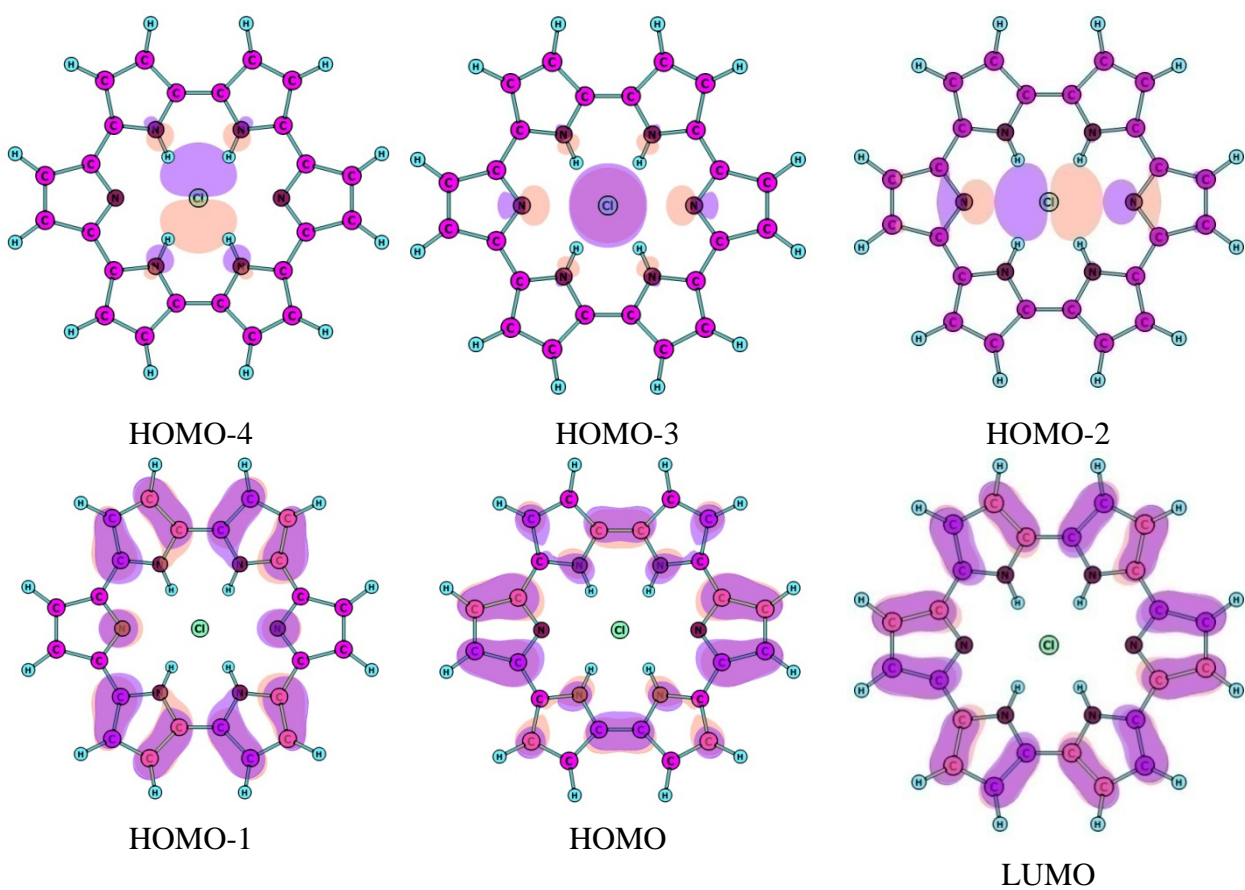


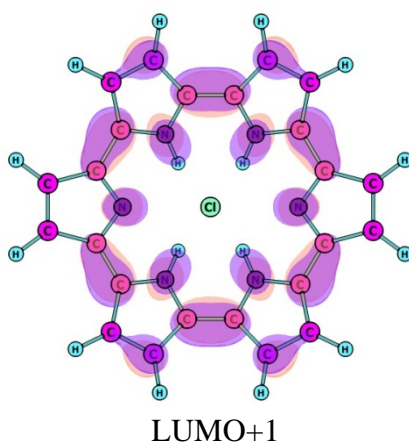
**Figure S5.** Schematic description of frontier orbitals of the  $I[Cl^-]$  complex calculated at the M062X/def2-TZVP level.



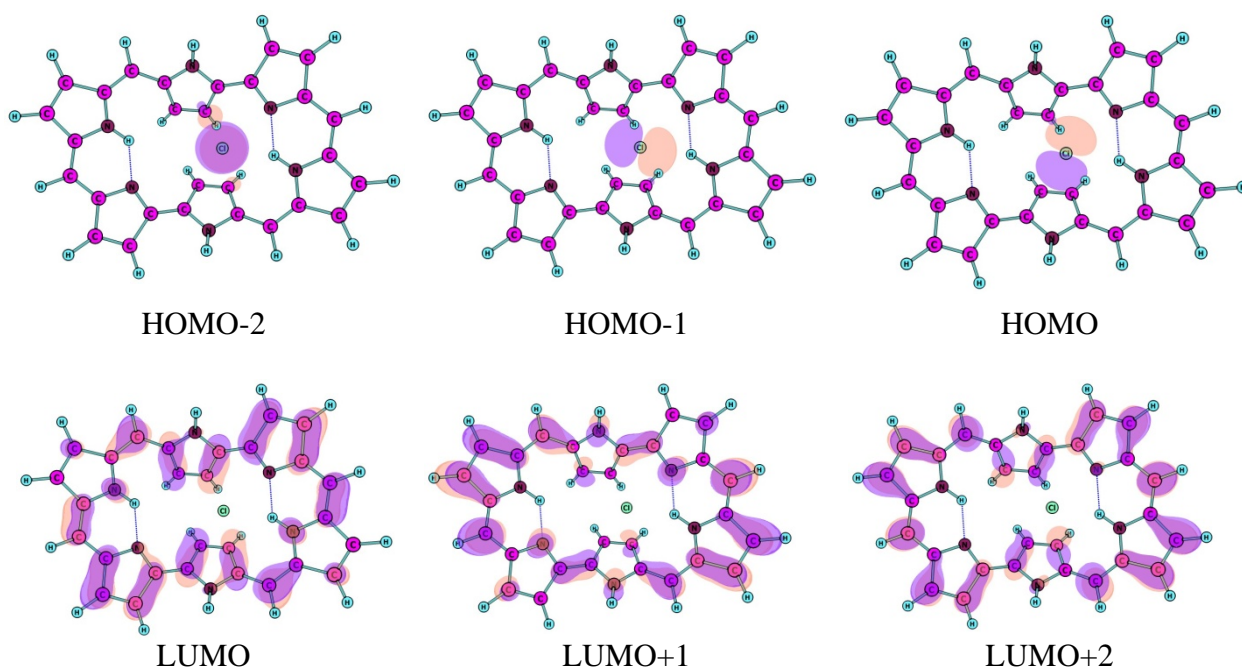


**Figure S6.** Schematic description of frontier orbitals of the  $\text{II}[\text{Cl}^-]$  complex calculated at the B3LYP/def2-TZVP level.

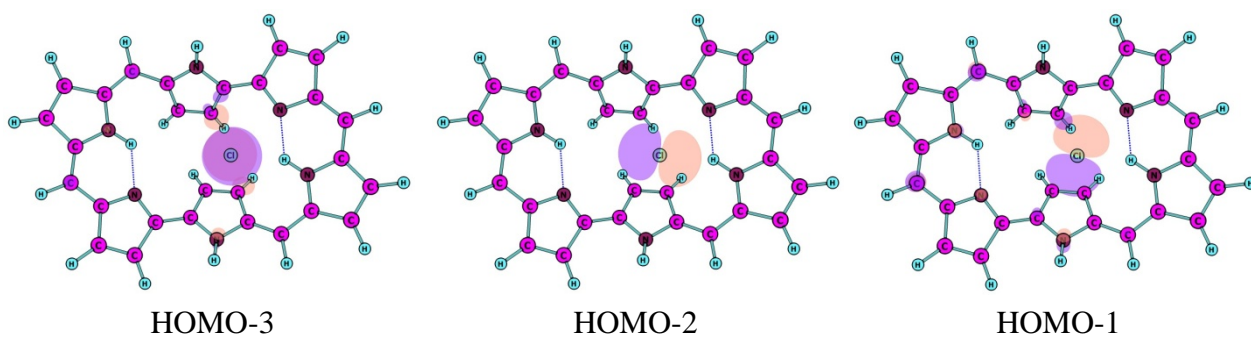


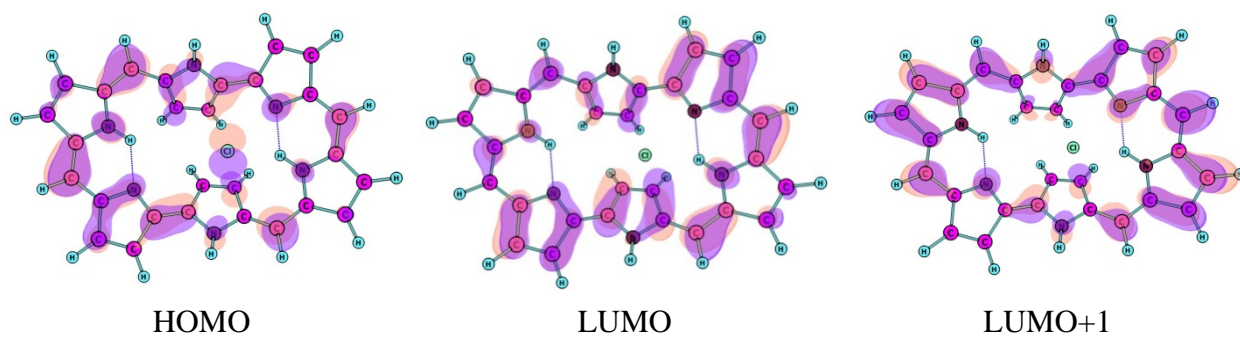


**Figure S7.** Schematic description of frontier orbitals of the  $\text{II}[\text{Cl}^-]$  complex calculated at the M062X/def2-TZVP level.

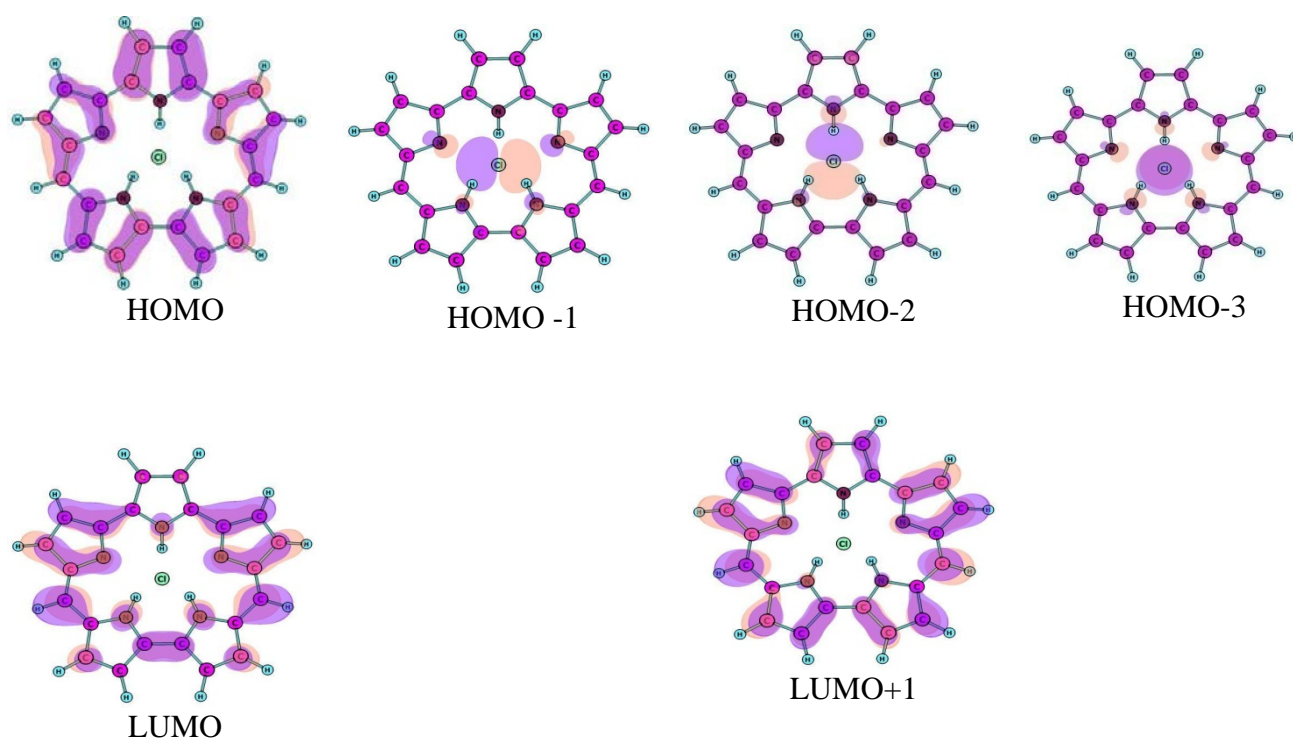


**Figure S8.** Schematic description of frontier orbitals of the  $\text{III}[\text{Cl}^-]$  complex calculated at the B3LYP/def2-TZVP level.

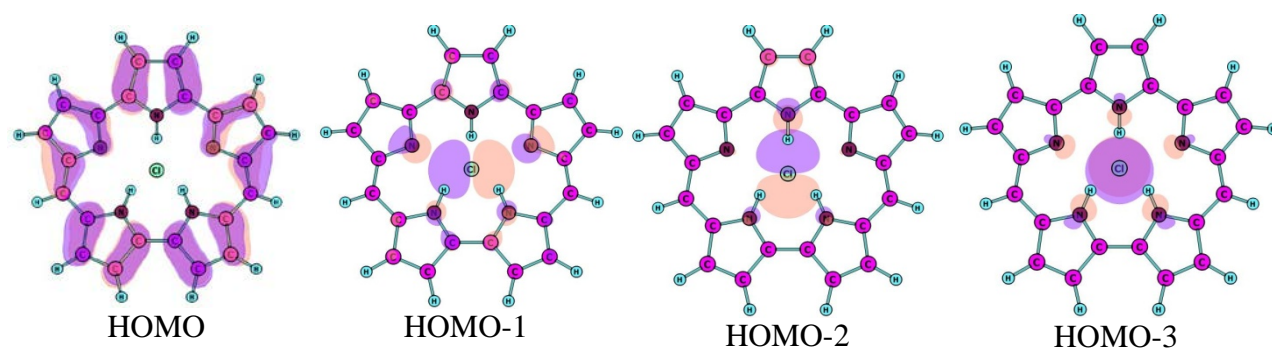


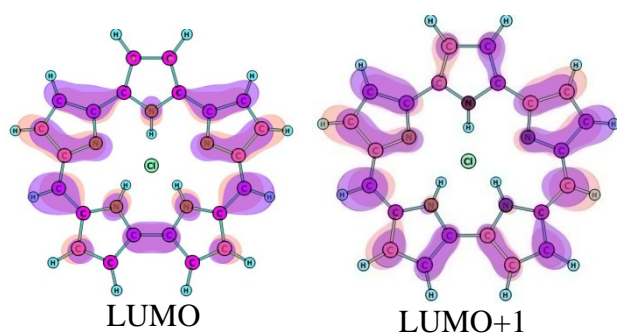


**Figure S9.** Schematic description of frontier orbitals of the III[Cl<sup>-</sup>] complex calculated at the M062X/def2-TZVP level.

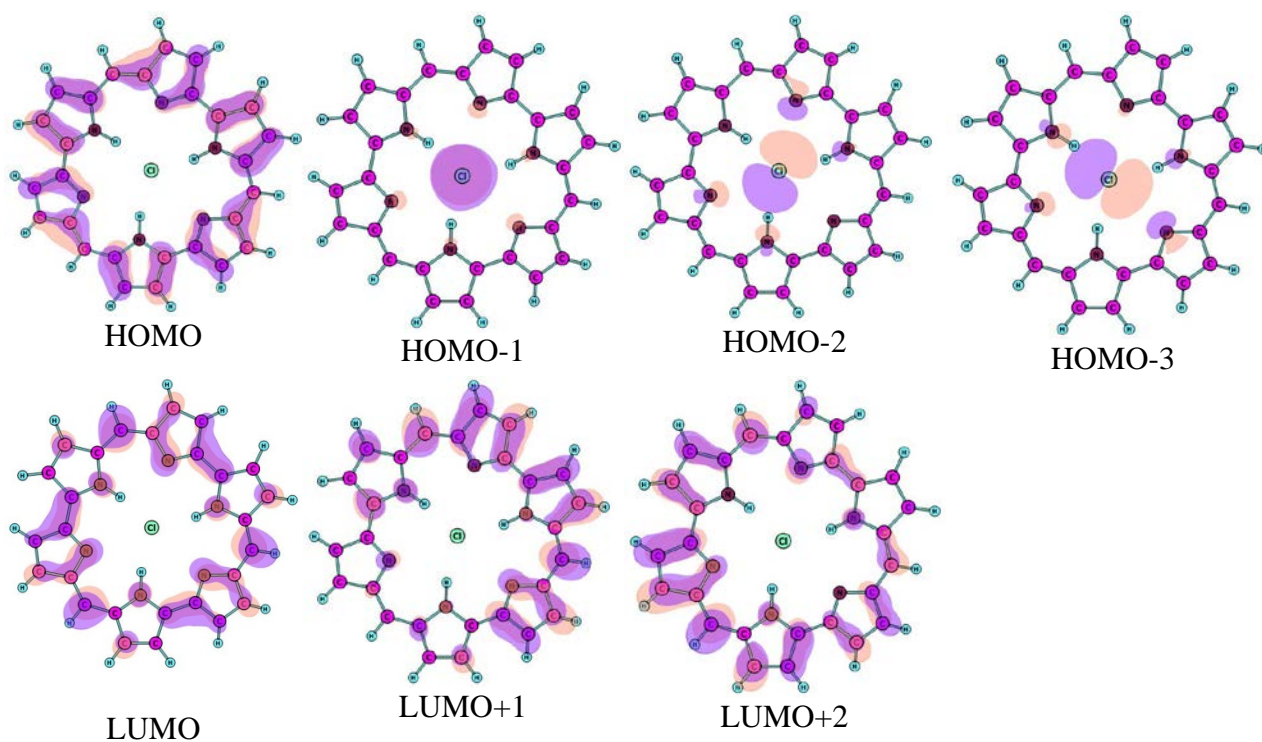


**Figure S10.** Schematic description of frontier orbitals of the IV[Cl<sup>-</sup>] complex calculated at the B3LYP/def2-TZVP level.

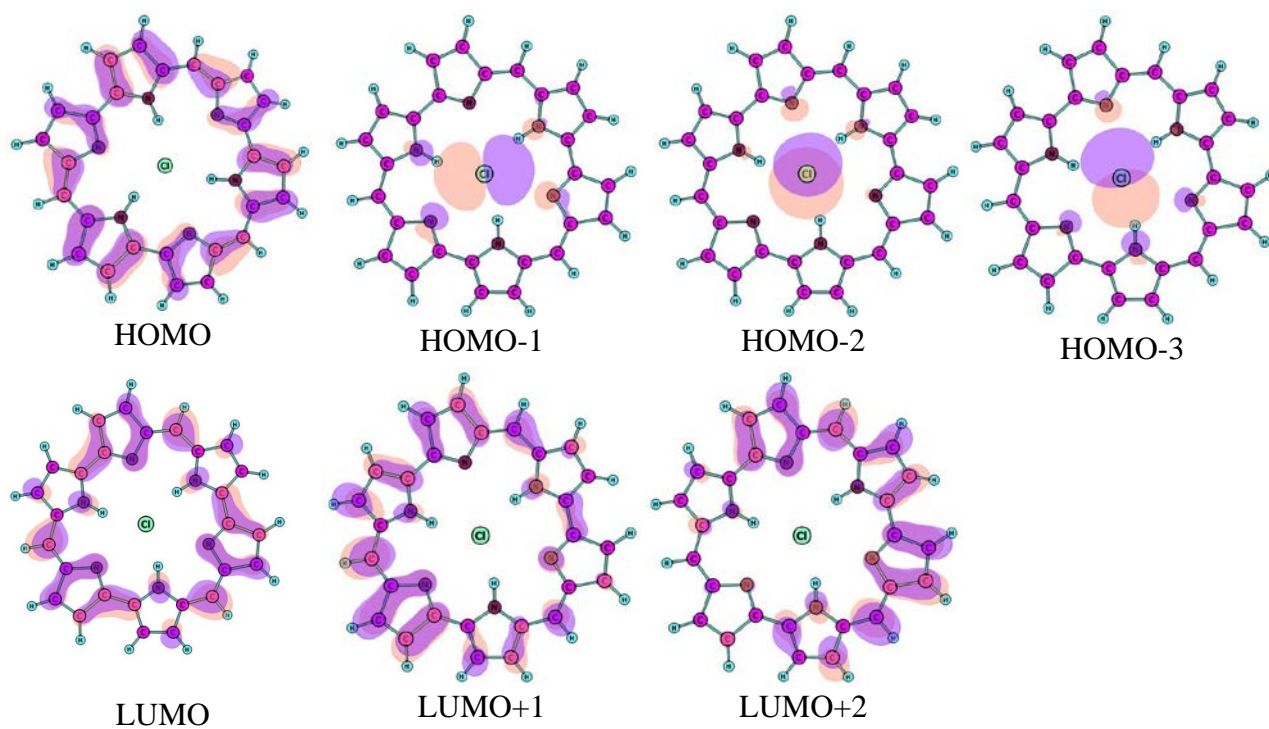




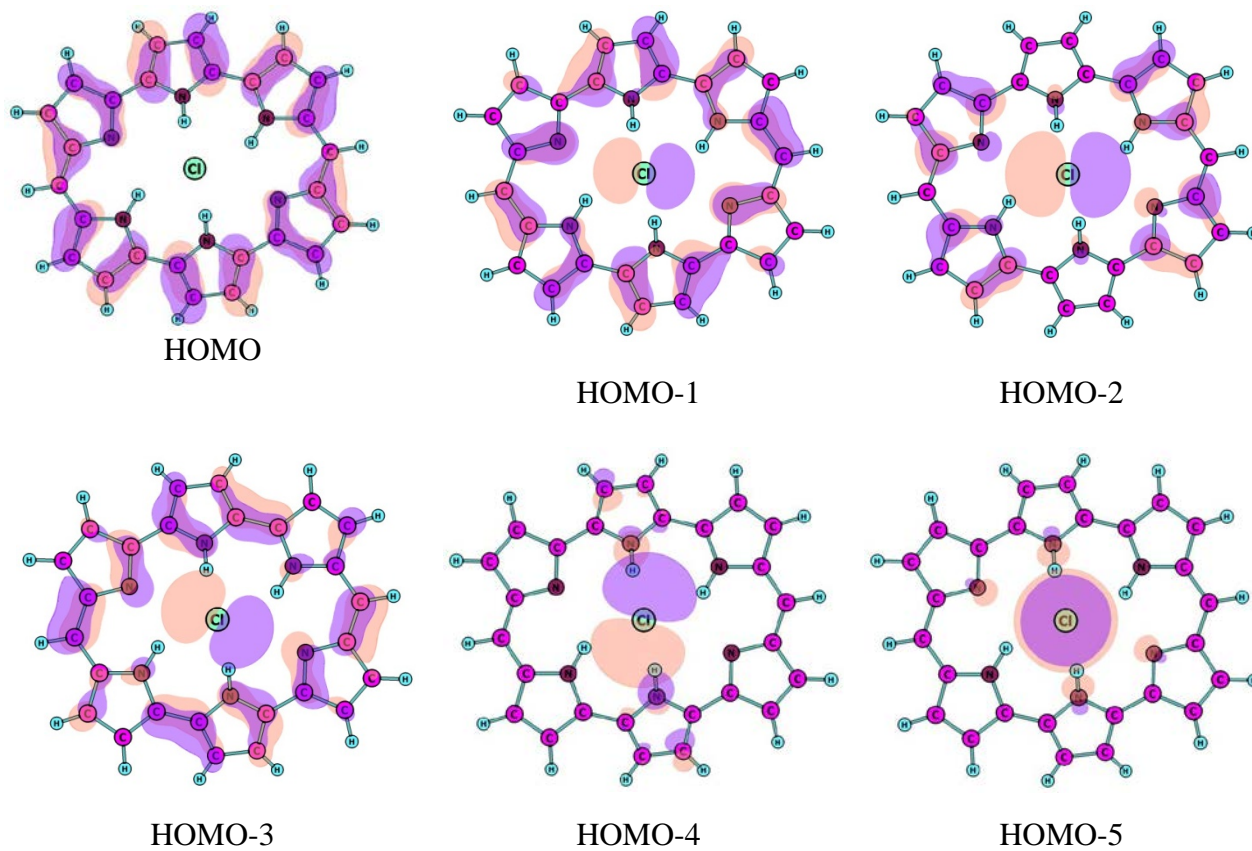
**Figure S11.** Schematic description of frontier orbitals of the IV[Cl<sup>-</sup>] complex calculated at the M062X/def2-TZVP level.

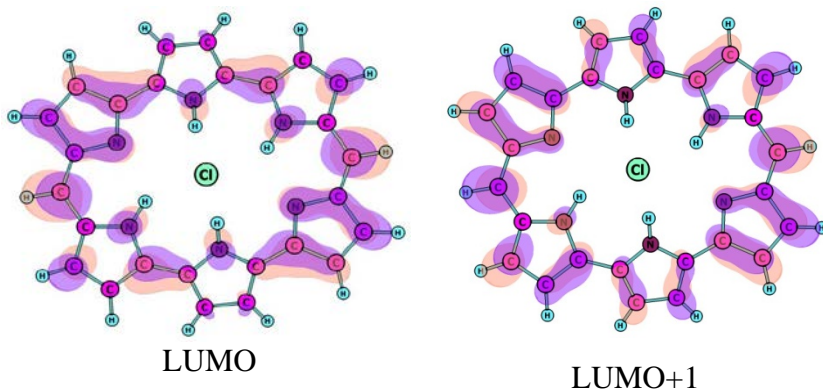


**Figure S12.** Schematic description of frontier orbitals of the V[Cl<sup>-</sup>] complex calculated at the B3LYP/def2-TZVP level.

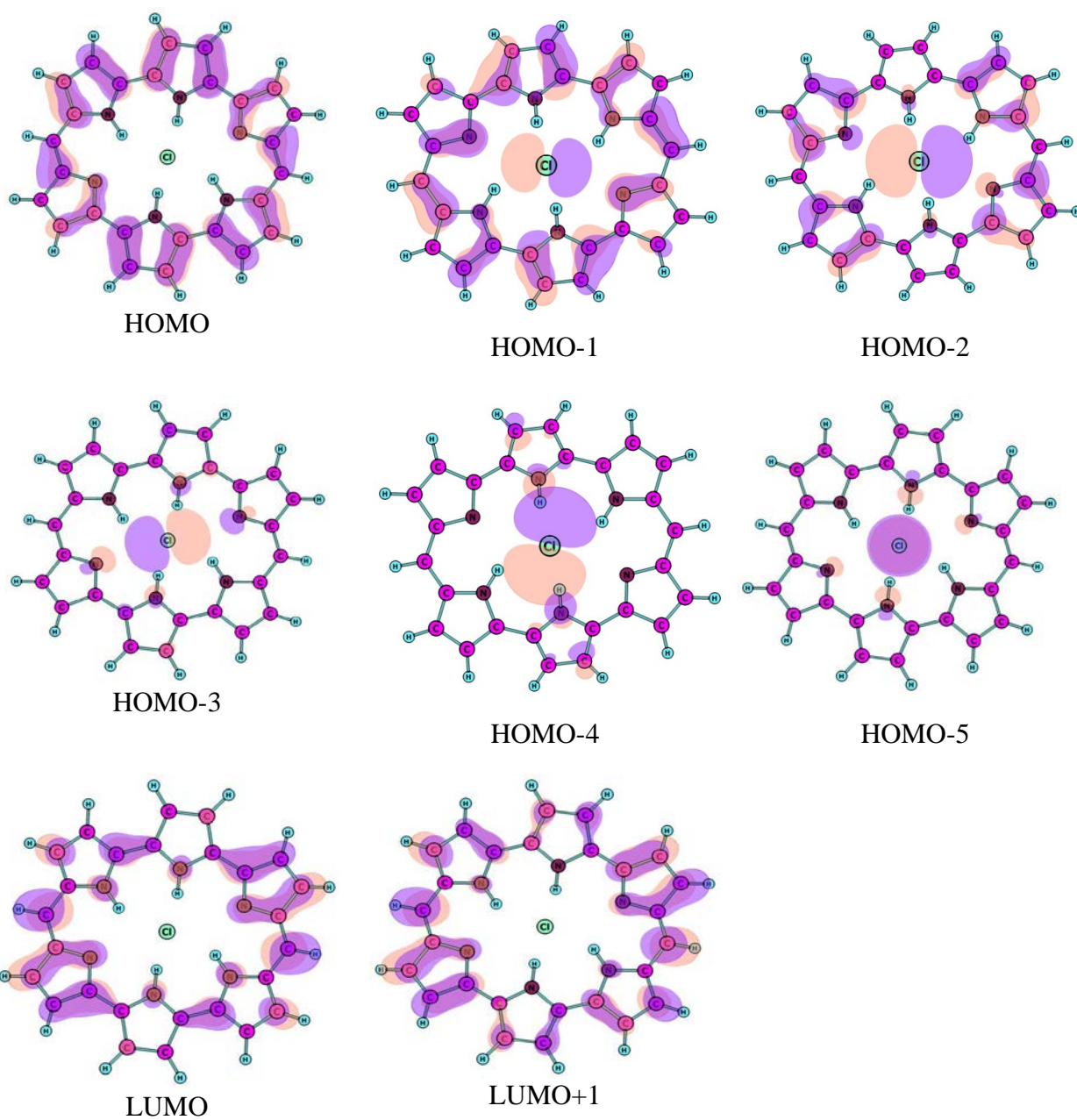


**FigureS13.** Schematic description of frontier orbitals of the  $V[Cl]^-$  complex calculated at the M062X/def2-TZVP level.

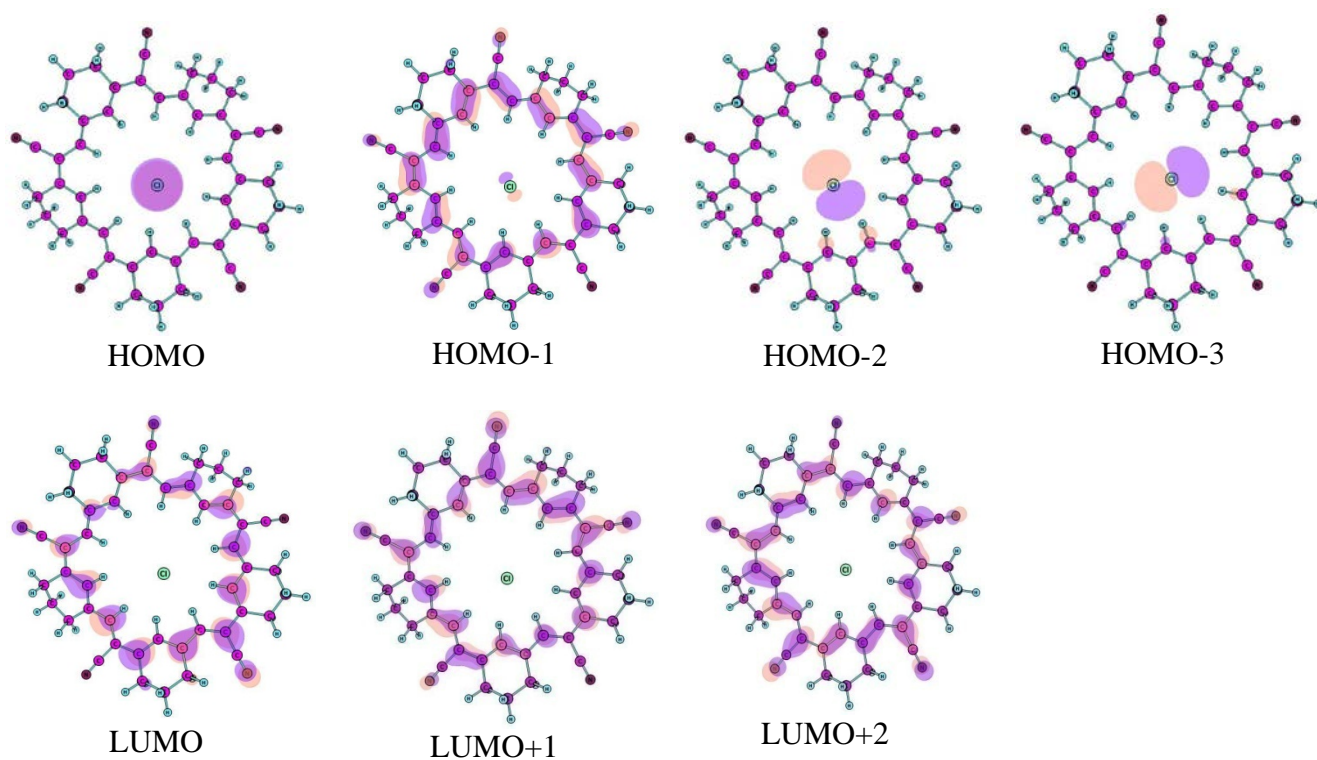




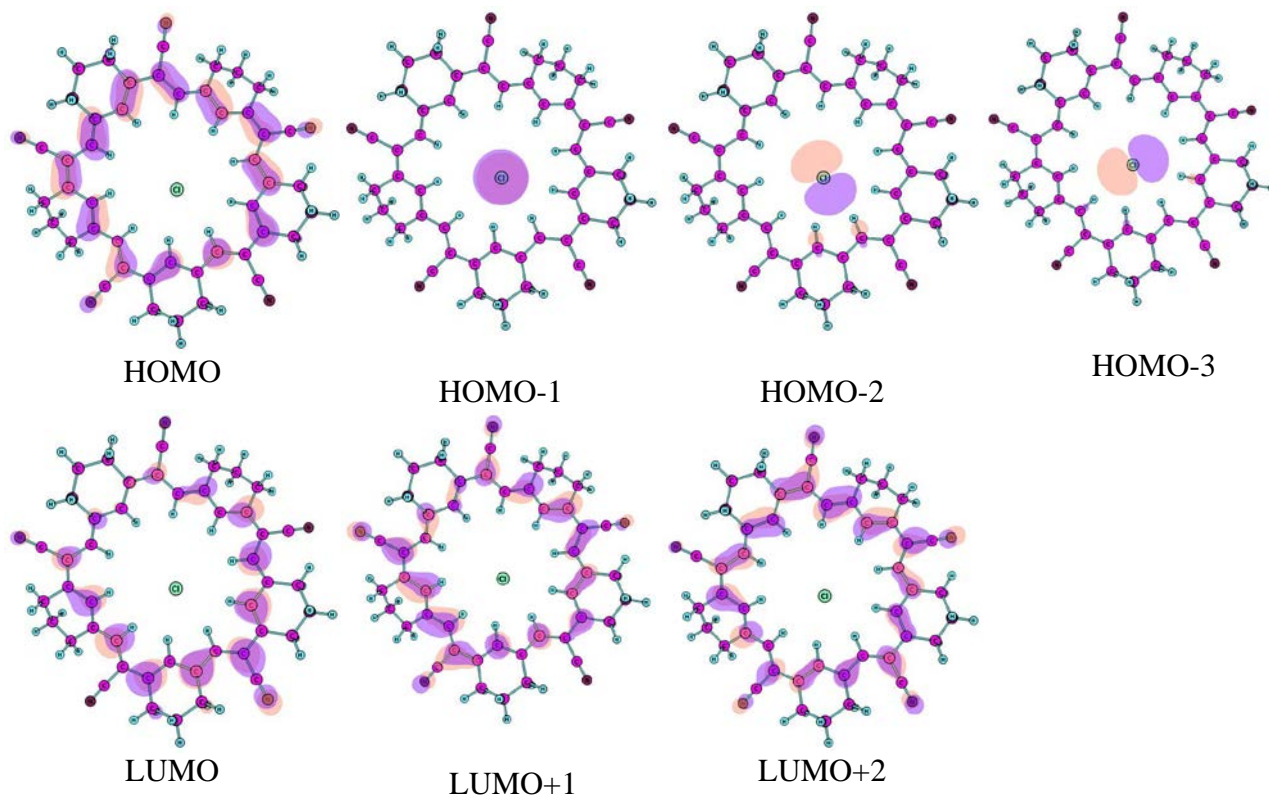
**FigureS14.** Schematic description of frontier orbitals of the VI[Cl<sup>-</sup>] complex calculated at the B3LYP/def2-TZVP level.



**FigureS15.** Schematic description of frontier orbitals of the VI[Cl<sup>-</sup>] complex calculated at the M062X/def2-TZVP level.

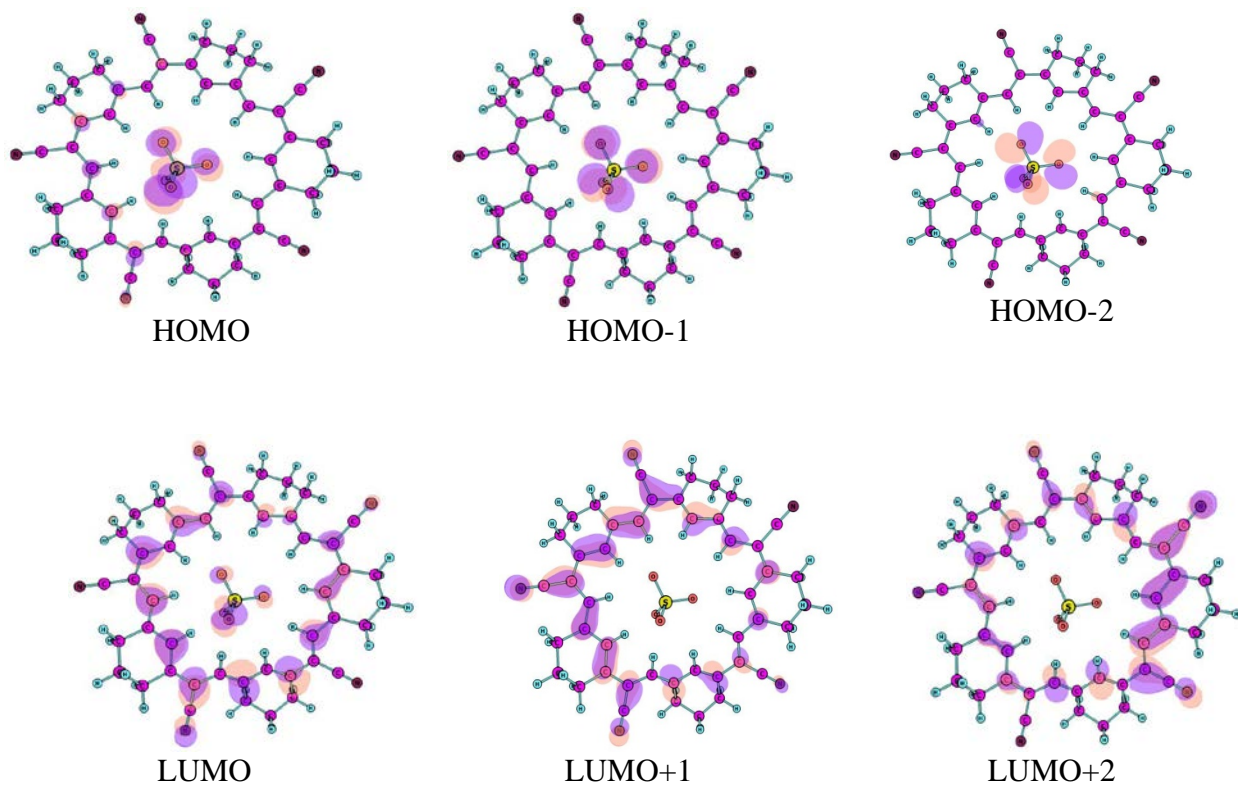


**FigureS16.** Schematic description of frontier orbitals of the VII[Cl<sup>-</sup>] complex calculated at the B3LYP/def2-TZVP level.

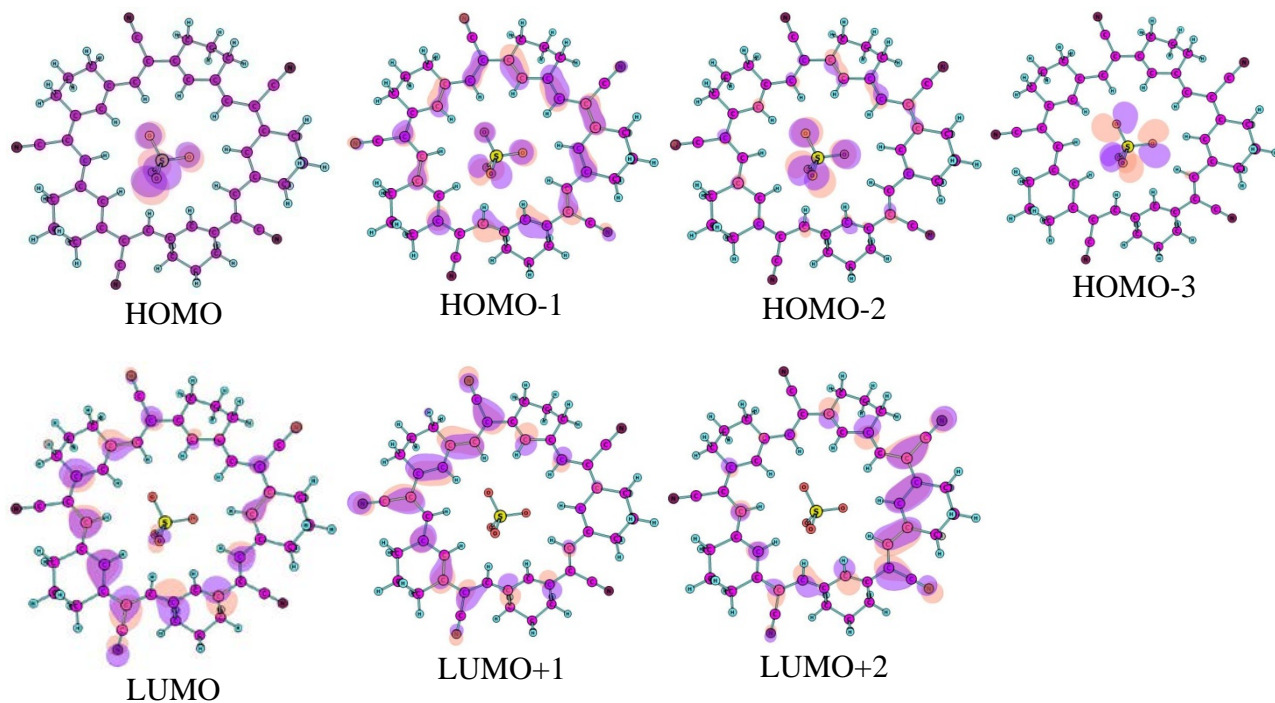


**Figure S17.** Schematic description of frontier orbitals of the VII[Cl<sup>-</sup>] complex calculated at the M062X/def2-TZVP level.





**Figure S18.** Schematic description of frontier orbitals of the  $\text{VII}[\text{SO}_4]^{2-}$  complex calculated at the B3LYP/def2-TZVP level.



**Figure S19.** Schematic description of frontier orbitals of the  $\text{VII}[\text{SO}_4]^{2-}$  complex calculated at the M062X/def2-TZVP level.

## Molecular structures

The Cartesian coordinates (in Å) of the atoms of the optimized molecular structures.

|   | <b>I (M06-2X)</b> |              |             |
|---|-------------------|--------------|-------------|
| N | -0.000069000      | -2.575546000 | 0.001715000 |
| C | 1.132108000       | -3.358906000 | 0.001778000 |
| C | 0.677092000       | -4.726125000 | 0.001872000 |
| C | -0.669998000      | -4.728382000 | 0.001860000 |
| C | -1.129605000      | -3.362715000 | 0.001757000 |
| C | 5.054569000       | -0.589753000 | 0.001595000 |
| C | 4.638319000       | -1.868438000 | 0.001682000 |
| C | 3.181419000       | -1.823056000 | 0.001676000 |
| N | 2.724807000       | -0.566889000 | 0.001590000 |
| C | 3.853366000       | 0.221715000  | 0.001540000 |
| N | -2.731939000      | -0.576117000 | 0.001541000 |
| C | -3.184178000      | -1.833861000 | 0.001617000 |
| C | -4.640902000      | -1.884332000 | 0.001599000 |
| C | -5.061614000      | -0.607083000 | 0.001499000 |
| C | -3.863236000      | 0.208545000  | 0.001468000 |
| C | -2.835643000      | 2.469964000  | 0.001331000 |
| C | -2.858686000      | 3.875384000  | 0.001234000 |
| C | -1.552877000      | 4.317828000  | 0.001219000 |
| C | -0.717408000      | 3.185140000  | 0.001304000 |
| N | -1.520046000      | 2.086827000  | 0.001372000 |
| C | 0.697324000       | 3.187546000  | 0.001317000 |
| C | 1.528921000       | 4.323081000  | 0.001245000 |
| C | 2.836232000       | 3.885095000  | 0.001286000 |
| C | 2.817996000       | 2.479617000  | 0.001383000 |
| N | 1.503724000       | 2.091982000  | 0.001401000 |
| C | -2.462468000      | -3.046041000 | 0.001714000 |
| C | 2.463884000       | -3.037701000 | 0.001760000 |
| C | -3.914250000      | 1.582191000  | 0.001375000 |
| C | 3.899641000       | 1.595527000  | 0.001448000 |
| H | -0.001733000      | -1.568879000 | 0.001640000 |
| H | 1.346397000       | -5.571283000 | 0.001937000 |
| H | -1.336447000      | -5.575802000 | 0.001913000 |
| H | 6.062296000       | -0.203994000 | 0.001571000 |
| H | 5.228582000       | -2.771787000 | 0.001741000 |
| H | -5.228039000      | -2.789705000 | 0.001650000 |
| H | -6.070657000      | -0.224774000 | 0.001452000 |
| H | -3.755729000      | 4.472900000  | 0.001185000 |
| H | -1.207854000      | 5.337725000  | 0.001153000 |
| H | -1.273886000      | 1.103341000  | 0.001440000 |
| H | 1.180398000       | 5.341771000  | 0.001171000 |
| H | 3.731253000       | 4.485646000  | 0.001252000 |
| H | 1.260956000       | 1.107659000  | 0.001467000 |
| H | -3.095717000      | -3.924883000 | 0.001765000 |
| H | 3.100107000       | -3.914391000 | 0.001821000 |
| H | -4.897094000      | 2.037046000  | 0.001327000 |
| H | 4.880898000       | 2.053804000  | 0.001420000 |

**II(M06-2X)**

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.679339000  | -2.335168000 | -0.071880000 |
| C | 2.961235000  | -3.711297000 | 0.075091000  |
| C | 1.751622000  | -4.397369000 | 0.098108000  |
| C | 0.709153000  | -3.452552000 | -0.026754000 |
| N | 1.325067000  | -2.246100000 | -0.140374000 |
| C | 4.737301000  | 0.685311000  | -0.016039000 |
| C | 4.737301000  | -0.685311000 | -0.016039000 |
| C | 3.359470000  | -1.085474000 | -0.109388000 |
| N | 2.567951000  | 0.000000000  | -0.177859000 |
| C | 3.359470000  | 1.085474000  | -0.109388000 |
| N | 1.325067000  | 2.246100000  | -0.140374000 |
| C | 0.709153000  | 3.452552000  | -0.026754000 |
| C | 1.751622000  | 4.397369000  | 0.098108000  |
| C | 2.961235000  | 3.711297000  | 0.075091000  |
| C | 2.679339000  | 2.335168000  | -0.071880000 |
| C | -0.709153000 | -3.452552000 | 0.026754000  |
| C | -1.751622000 | -4.397369000 | -0.098108000 |
| C | -2.961235000 | -3.711297000 | -0.075091000 |
| C | -2.679339000 | -2.335168000 | 0.071880000  |
| N | -1.325067000 | -2.246100000 | 0.140374000  |
| N | -1.325067000 | 2.246100000  | 0.140374000  |
| C | -2.679339000 | 2.335168000  | 0.071880000  |
| C | -2.961235000 | 3.711297000  | -0.075091000 |
| C | -1.751622000 | 4.397369000  | -0.098108000 |
| C | -0.709153000 | 3.452552000  | 0.026754000  |
| N | -2.567951000 | 0.000000000  | 0.177859000  |
| C | -3.359470000 | -1.085474000 | 0.109388000  |
| C | -4.737301000 | -0.685311000 | 0.016039000  |
| C | -4.737301000 | 0.685311000  | 0.016039000  |
| C | -3.359470000 | 1.085474000  | 0.109388000  |
| H | 3.943539000  | -4.142669000 | 0.173974000  |
| H | 1.616099000  | -5.458348000 | 0.228722000  |
| H | 0.916241000  | -1.345445000 | -0.325612000 |
| H | 5.592751000  | 1.338747000  | 0.050204000  |
| H | 5.592751000  | -1.338747000 | 0.050204000  |
| H | 0.916241000  | 1.345445000  | -0.325612000 |
| H | 1.616099000  | 5.458348000  | 0.228723000  |
| H | 3.943539000  | 4.142669000  | 0.173974000  |
| H | -1.616099000 | -5.458348000 | -0.228722000 |
| H | -3.943539000 | -4.142669000 | -0.173974000 |
| H | -0.916241000 | -1.345445000 | 0.325612000  |
| H | -0.916241000 | 1.345445000  | 0.325612000  |
| H | -3.943539000 | 4.142669000  | -0.173974000 |
| H | -1.616099000 | 5.458348000  | -0.228723000 |
| H | -5.592751000 | -1.338747000 | -0.050204000 |
| H | -5.592751000 | 1.338747000  | -0.050204000 |

**III(M06-2X)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 1.878481000 | 0.026887000 | 0.000000000 |
|---|-------------|-------------|-------------|

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 1.054383000  | 1.094493000  | 0.000000000 |
| C | 1.813494000  | 2.271402000  | 0.000000000 |
| N | 3.144987000  | 1.860276000  | 0.000000000 |
| C | 3.214745000  | 0.455510000  | 0.000000000 |
| C | 4.112653000  | -1.872666000 | 0.000000000 |
| C | 5.175780000  | -2.841738000 | 0.000000000 |
| C | 4.640821000  | -4.107239000 | 0.000000000 |
| C | 3.214745000  | -3.979156000 | 0.000000000 |
| N | 2.963496000  | -2.632534000 | 0.000000000 |
| C | -3.214745000 | -0.455510000 | 0.000000000 |
| C | -1.878481000 | -0.026887000 | 0.000000000 |
| C | -1.054383000 | -1.094493000 | 0.000000000 |
| C | -1.813494000 | -2.271402000 | 0.000000000 |
| N | -3.144987000 | -1.860276000 | 0.000000000 |
| N | -0.282061000 | 3.383477000  | 0.000000000 |
| C | -0.793746000 | 4.635257000  | 0.000000000 |
| C | 0.293722000  | 5.604856000  | 0.000000000 |
| C | 1.457570000  | 4.892498000  | 0.000000000 |
| C | 1.078372000  | 3.495673000  | 0.000000000 |
| N | -2.963496000 | 2.632534000  | 0.000000000 |
| C | -4.112653000 | 1.872666000  | 0.000000000 |
| C | -5.175780000 | 2.841738000  | 0.000000000 |
| C | -4.640821000 | 4.107239000  | 0.000000000 |
| C | -3.214745000 | 3.979156000  | 0.000000000 |
| C | -0.293722000 | -5.604856000 | 0.000000000 |
| C | -1.457570000 | -4.892498000 | 0.000000000 |
| C | -1.078372000 | -3.495673000 | 0.000000000 |
| N | 0.282061000  | -3.383477000 | 0.000000000 |
| C | 0.793746000  | -4.635257000 | 0.000000000 |
| C | 2.178256000  | -4.922792000 | 0.000000000 |
| C | 4.274676000  | -0.463581000 | 0.000000000 |
| C | -4.274676000 | 0.463581000  | 0.000000000 |
| C | -2.178256000 | 4.922792000  | 0.000000000 |
| H | 1.568815000  | -0.981513000 | 0.000000000 |
| H | -0.001614000 | 1.116743000  | 0.000000000 |
| H | 3.943579000  | 2.474069000  | 0.000000000 |
| H | 6.225306000  | -2.580483000 | 0.000000000 |
| H | 5.180832000  | -5.043378000 | 0.000000000 |
| H | -1.568815000 | 0.981513000  | 0.000000000 |
| H | 0.001614000  | -1.116743000 | 0.000000000 |
| H | -3.943579000 | -2.474069000 | 0.000000000 |
| H | 0.180585000  | 6.681314000  | 0.000000000 |
| H | 2.466614000  | 5.282549000  | 0.000000000 |
| H | -6.225306000 | 2.580483000  | 0.000000000 |
| H | -5.180832000 | 5.043378000  | 0.000000000 |
| H | -0.180585000 | -6.681314000 | 0.000000000 |
| H | -2.466614000 | -5.282549000 | 0.000000000 |
| H | 2.471311000  | -5.967996000 | 0.000000000 |
| H | 5.304972000  | -0.121862000 | 0.000000000 |
| H | -5.304972000 | 0.121862000  | 0.000000000 |
| H | -2.471311000 | 5.967996000  | 0.000000000 |
| H | -1.978959000 | 2.400232000  | 0.000000000 |

|   |             |              |             |
|---|-------------|--------------|-------------|
| H | 1.978959000 | -2.400232000 | 0.000000000 |
|---|-------------|--------------|-------------|

**IV(M06-2X)**

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 0.000000000  | 0.109530000  | 2.169704000  |
| C | -1.121359000 | 0.024931000  | 2.917343000  |
| C | -0.708109000 | -0.105331000 | 4.237045000  |
| C | 0.708109000  | -0.105331000 | 4.237045000  |
| C | 1.121359000  | 0.024931000  | 2.917343000  |
| C | -4.483695000 | 0.010169000  | 1.434996000  |
| C | -3.748942000 | 0.009846000  | 2.574357000  |
| C | -2.359153000 | 0.026200000  | 2.151720000  |
| N | -2.252550000 | 0.033953000  | 0.846251000  |
| C | -3.542442000 | 0.022234000  | 0.331187000  |
| N | 2.252550000  | 0.033953000  | 0.846251000  |
| C | 2.359153000  | 0.026200000  | 2.151720000  |
| C | 3.748942000  | 0.009846000  | 2.574357000  |
| C | 4.483695000  | 0.010169000  | 1.434996000  |
| C | 3.542442000  | 0.022234000  | 0.331187000  |
| C | 2.790850000  | -0.004677000 | -2.031629000 |
| C | 2.915412000  | 0.003369000  | -3.420403000 |
| C | 1.626220000  | -0.005423000 | -3.965289000 |
| C | 0.724428000  | -0.020864000 | -2.902931000 |
| N | 1.447147000  | -0.021069000 | -1.757956000 |
| C | -0.724428000 | -0.020864000 | -2.902931000 |
| C | -1.626220000 | -0.005423000 | -3.965289000 |
| C | -2.915412000 | 0.003369000  | -3.420403000 |
| C | -2.790850000 | -0.004677000 | -2.031629000 |
| N | -1.447147000 | -0.021069000 | -1.757956000 |
| C | 3.787217000  | 0.006538000  | -1.009989000 |
| C | -3.787217000 | 0.006538000  | -1.009989000 |
| H | 0.000000000  | 0.220152000  | 1.172966000  |
| H | -1.349669000 | -0.204218000 | 5.096685000  |
| H | 1.349669000  | -0.204218000 | 5.096685000  |
| H | -5.558783000 | 0.000710000  | 1.341952000  |
| H | -4.102527000 | 0.003043000  | 3.592925000  |
| H | 4.102527000  | 0.003043000  | 3.592925000  |
| H | 5.558783000  | 0.000710000  | 1.341952000  |
| H | 3.847932000  | 0.017794000  | -3.960699000 |
| H | 1.360665000  | 0.001071000  | -5.009021000 |
| H | 1.143332000  | -0.039321000 | -0.790556000 |
| H | -1.360665000 | 0.001071000  | -5.009021000 |
| H | -3.847932000 | 0.017794000  | -3.960699000 |
| H | -1.143332000 | -0.039321000 | -0.790556000 |
| H | 4.817018000  | 0.000275000  | -1.347324000 |
| H | -4.817018000 | 0.000275000  | -1.347324000 |

**V(M06-2X)**

|   |             |             |             |
|---|-------------|-------------|-------------|
| C | 3.592874000 | 1.148300000 | 0.000000000 |
| C | 4.728007000 | 2.066997000 | 0.000000000 |
| C | 4.195188000 | 3.301579000 | 0.000000000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 2.755173000  | 3.124862000  | 0.000000000 |
| N | 2.437543000  | 1.764606000  | 0.000000000 |
| C | 4.742058000  | -2.313604000 | 0.000000000 |
| C | 5.010454000  | -0.947690000 | 0.000000000 |
| C | 3.786346000  | -0.283122000 | 0.000000000 |
| N | 2.801451000  | -1.218474000 | 0.000000000 |
| C | 3.357954000  | -2.468687000 | 0.000000000 |
| N | 0.308097000  | -2.994492000 | 0.000000000 |
| C | -0.802730000 | -3.687604000 | 0.000000000 |
| C | -0.574079000 | -5.129705000 | 0.000000000 |
| C | 0.761444000  | -5.285039000 | 0.000000000 |
| C | 1.328058000  | -3.949134000 | 0.000000000 |
| C | 0.458821000  | 4.143562000  | 0.000000000 |
| C | -0.367593000 | 5.264715000  | 0.000000000 |
| C | -1.684730000 | 4.813817000  | 0.000000000 |
| C | -1.647973000 | 3.421679000  | 0.000000000 |
| N | -0.345256000 | 3.036340000  | 0.000000000 |
| N | -2.455176000 | -1.818286000 | 0.000000000 |
| C | -3.816063000 | -1.673863000 | 0.000000000 |
| C | -4.375150000 | -2.949159000 | 0.000000000 |
| C | -3.327519000 | -3.865799000 | 0.000000000 |
| C | -2.139079000 | -3.139355000 | 0.000000000 |
| N | -2.746004000 | 1.229979000  | 0.000000000 |
| C | -2.790772000 | 2.538451000  | 0.000000000 |
| C | -4.154360000 | 3.061469000  | 0.000000000 |
| C | -4.956319000 | 1.982589000  | 0.000000000 |
| C | -4.082642000 | 0.824222000  | 0.000000000 |
| H | 5.769594000  | 1.791121000  | 0.000000000 |
| H | 4.703384000  | 4.253468000  | 0.000000000 |
| H | 5.450639000  | -3.125602000 | 0.000000000 |
| H | 5.977213000  | -0.475221000 | 0.000000000 |
| H | -1.333634000 | -5.893798000 | 0.000000000 |
| H | 1.332483000  | -6.200669000 | 0.000000000 |
| H | -0.018761000 | 6.284487000  | 0.000000000 |
| H | -2.577880000 | 5.414166000  | 0.000000000 |
| H | 0.006185000  | 2.087944000  | 0.000000000 |
| H | -1.807428000 | -1.041553000 | 0.000000000 |
| H | -5.432913000 | -3.155670000 | 0.000000000 |
| H | -3.402513000 | -4.939215000 | 0.000000000 |
| H | -4.435935000 | 4.101562000  | 0.000000000 |
| H | -6.034723000 | 1.945925000  | 0.000000000 |
| C | 2.660620000  | -3.704493000 | 0.000000000 |
| H | 3.307084000  | -4.574977000 | 0.000000000 |
| H | 1.804720000  | -1.047284000 | 0.000000000 |
| C | -4.537243000 | -0.451967000 | 0.000000000 |
| H | -5.614264000 | -0.577100000 | 0.000000000 |
| C | 1.877540000  | 4.157208000  | 0.000000000 |
| H | 2.307806000  | 5.152513000  | 0.000000000 |

**VI(M06-2X)**

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 0.946225000  | 4.522501000 | -0.349989000 |
| C | -0.457618000 | 4.598831000 | -0.390002000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.950577000 | 3.327218000  | -0.164448000 |
| N | 0.122613000  | 2.497745000  | 0.003482000  |
| C | 1.285691000  | 3.205292000  | -0.094359000 |
| C | 2.590343000  | 2.607970000  | 0.051244000  |
| C | 3.823544000  | 3.234336000  | 0.216644000  |
| C | 4.792763000  | 2.231772000  | 0.299096000  |
| C | 4.143299000  | 1.004609000  | 0.190282000  |
| N | 2.804292000  | 1.269706000  | 0.043909000  |
| C | -1.285691000 | -3.205292000 | -0.094359000 |
| C | -0.946225000 | -4.522501000 | -0.349989000 |
| C | 0.457618000  | -4.598831000 | -0.390002000 |
| C | 0.950577000  | -3.327218000 | -0.164448000 |
| N | -0.122613000 | -2.497745000 | 0.003482000  |
| N | -2.574679000 | 1.548640000  | 0.014039000  |
| C | -3.966694000 | 1.468836000  | 0.095212000  |
| C | -4.531657000 | 2.800195000  | 0.038205000  |
| C | -3.493457000 | 3.656091000  | -0.083883000 |
| C | -2.300339000 | 2.828372000  | -0.087282000 |
| N | -2.804292000 | -1.269706000 | 0.043909000  |
| C | -2.590343000 | -2.607970000 | 0.051244000  |
| C | -3.823544000 | -3.234336000 | 0.216644000  |
| C | -4.792763000 | -2.231772000 | 0.299096000  |
| C | -4.143299000 | -1.004609000 | 0.190282000  |
| C | 4.531657000  | -2.800195000 | 0.038205000  |
| C | 3.493457000  | -3.656091000 | -0.083883000 |
| C | 2.300339000  | -2.828372000 | -0.087282000 |
| N | 2.574679000  | -1.548640000 | 0.014039000  |
| C | 3.966694000  | -1.468836000 | 0.095212000  |
| C | 4.673683000  | -0.309092000 | 0.191485000  |
| C | -4.673683000 | 0.309092000  | 0.191485000  |
| H | 1.647805000  | 5.324010000  | -0.508723000 |
| H | -1.052646000 | 5.476026000  | -0.581384000 |
| H | 0.018508000  | 1.534005000  | 0.272182000  |
| H | 3.974577000  | 4.298440000  | 0.281869000  |
| H | 5.854730000  | 2.360466000  | 0.431869000  |
| H | -1.647805000 | -5.324010000 | -0.508723000 |
| H | 1.052646000  | -5.476026000 | -0.581384000 |
| H | -0.018508000 | -1.534005000 | 0.272182000  |
| H | -5.585214000 | 3.029806000  | 0.082612000  |
| H | -3.516169000 | 4.731845000  | -0.151170000 |
| H | -3.974577000 | -4.298440000 | 0.281869000  |
| H | -5.854730000 | -2.360466000 | 0.431869000  |
| H | 5.585214000  | -3.029806000 | 0.082612000  |
| H | 3.516169000  | -4.731845000 | -0.151170000 |
| H | 5.752435000  | -0.384301000 | 0.264183000  |
| H | -5.752435000 | 0.384301000  | 0.264183000  |
| H | -2.150916000 | -0.508793000 | -0.102491000 |
| H | 2.150916000  | 0.508793000  | -0.102491000 |

**I[Cl<sup>-</sup>] (B3LYP)**

|   |              |              |             |
|---|--------------|--------------|-------------|
| N | -0.000142000 | -2.551202000 | 0.012360000 |
|---|--------------|--------------|-------------|

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 1.130256000  | -3.335054000 | 0.122891000  |
| C  | 0.682065000  | -4.683314000 | 0.330269000  |
| C  | -0.675010000 | -4.685714000 | 0.329876000  |
| C  | -1.127825000 | -3.339042000 | 0.122322000  |
| C  | 5.118520000  | -0.606631000 | -0.089622000 |
| C  | 4.700616000  | -1.892421000 | -0.065287000 |
| C  | 3.239123000  | -1.847452000 | 0.011480000  |
| N  | 2.802191000  | -0.579237000 | 0.037502000  |
| C  | 3.910838000  | 0.206326000  | -0.029300000 |
| N  | -2.809096000 | -0.588968000 | 0.037585000  |
| C  | -3.241694000 | -1.858638000 | 0.010632000  |
| C  | -4.702996000 | -1.908553000 | -0.066832000 |
| C  | -5.125265000 | -0.624179000 | -0.090606000 |
| C  | -3.920364000 | 0.192852000  | -0.029476000 |
| C  | -2.832137000 | 2.450812000  | -0.007011000 |
| C  | -2.865812000 | 3.857048000  | 0.186510000  |
| C  | -1.567396000 | 4.314874000  | 0.202299000  |
| C  | -0.717104000 | 3.198003000  | 0.001794000  |
| N  | -1.510673000 | 2.095111000  | -0.118783000 |
| C  | 0.697328000  | 3.200457000  | 0.001674000  |
| C  | 1.543807000  | 4.320265000  | 0.201899000  |
| C  | 2.843794000  | 3.866924000  | 0.185906000  |
| C  | 2.814922000  | 2.460552000  | -0.007396000 |
| N  | 1.494683000  | 2.100283000  | -0.118850000 |
| C  | -2.483510000 | -3.039297000 | 0.077563000  |
| C  | 2.484928000  | -3.030648000 | 0.078620000  |
| C  | -3.926714000 | 1.581452000  | -0.025008000 |
| C  | 3.912461000  | 1.594940000  | -0.025224000 |
| H  | -0.001797000 | -1.602571000 | -0.403792000 |
| H  | 1.347717000  | -5.519308000 | 0.478253000  |
| H  | -1.337795000 | -5.524047000 | 0.477498000  |
| H  | 6.129814000  | -0.231243000 | -0.151344000 |
| H  | 5.300386000  | -2.790701000 | -0.099371000 |
| H  | -5.299671000 | -2.808859000 | -0.101714000 |
| H  | -6.137788000 | -0.252159000 | -0.152625000 |
| H  | -3.766096000 | 4.434192000  | 0.327921000  |
| H  | -1.234713000 | 5.327905000  | 0.357184000  |
| H  | -1.188600000 | 1.178208000  | -0.473484000 |
| H  | 1.207679000  | 5.332185000  | 0.356594000  |
| H  | 3.742113000  | 4.447202000  | 0.326986000  |
| H  | 1.175782000  | 1.182199000  | -0.473217000 |
| H  | -3.093755000 | -3.935117000 | 0.127267000  |
| H  | 3.098200000  | -3.924362000 | 0.128960000  |
| H  | -4.897543000 | 2.063677000  | -0.009315000 |
| H  | 4.881632000  | 2.080492000  | -0.009611000 |
| Cl | -0.005145000 | -0.007349000 | -1.913889000 |

**I[Cl<sup>-</sup>] (M06-2X)**

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 0.006394000 | -2.527193000 | -0.033646000 |
| C | 1.132939000 | -3.310951000 | -0.122824000 |
| C | 0.682186000 | -4.672427000 | -0.307935000 |



|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -0.663176000 | -4.674571000 | -0.306270000 |
| C  | -1.117817000 | -3.314549000 | -0.120097000 |
| C  | 5.106830000  | -0.601289000 | 0.140712000  |
| C  | 4.684504000  | -1.880119000 | 0.114466000  |
| C  | 3.224304000  | -1.824108000 | 0.012891000  |
| N  | 2.787441000  | -0.572780000 | -0.023120000 |
| C  | 3.904248000  | 0.213788000  | 0.059080000  |
| N  | -2.781236000 | -0.581679000 | -0.017209000 |
| C  | -3.213793000 | -1.834490000 | 0.019743000  |
| C  | -4.673611000 | -1.895455000 | 0.123594000  |
| C  | -5.100288000 | -0.618051000 | 0.150080000  |
| C  | -3.900649000 | 0.201101000  | 0.066354000  |
| C  | -2.818135000 | 2.445855000  | 0.014306000  |
| C  | -2.852586000 | 3.841417000  | -0.179295000 |
| C  | -1.548947000 | 4.292828000  | -0.208125000 |
| C  | -0.714765000 | 3.173638000  | -0.014836000 |
| N  | -1.504135000 | 2.080063000  | 0.110127000  |
| C  | 0.708352000  | 3.175888000  | -0.016124000 |
| C  | 1.538577000  | 4.297812000  | -0.210606000 |
| C  | 2.843703000  | 3.850606000  | -0.183808000 |
| C  | 2.814074000  | 2.454941000  | 0.009664000  |
| N  | 1.501409000  | 2.084828000  | 0.107534000  |
| C  | -2.460491000 | -3.028969000 | -0.063459000 |
| C  | 2.474776000  | -3.021044000 | -0.069238000 |
| C  | -3.917271000 | 1.575118000  | 0.057218000  |
| C  | 3.916147000  | 1.587869000  | 0.050449000  |
| H  | 0.005409000  | -1.568860000 | 0.356877000  |
| H  | 1.354839000  | -5.506174000 | -0.434620000 |
| H  | -1.333466000 | -5.510481000 | -0.431249000 |
| H  | 6.115026000  | -0.221783000 | 0.217065000  |
| H  | 5.272160000  | -2.785400000 | 0.158466000  |
| H  | -5.258095000 | -2.802721000 | 0.168762000  |
| H  | -6.109653000 | -0.241931000 | 0.227733000  |
| H  | -3.754668000 | 4.418629000  | -0.306244000 |
| H  | -1.205517000 | 5.302318000  | -0.360747000 |
| H  | -1.185749000 | 1.151932000  | 0.435069000  |
| H  | 1.191628000  | 5.306204000  | -0.362514000 |
| H  | 3.743703000  | 4.430766000  | -0.312145000 |
| H  | 1.186499000  | 1.155771000  | 0.433501000  |
| H  | -3.073755000 | -3.922409000 | -0.106679000 |
| H  | 3.090841000  | -3.912490000 | -0.113978000 |
| H  | -4.888959000 | 2.056296000  | 0.064570000  |
| H  | 4.886186000  | 2.072396000  | 0.056355000  |
| Cl | 0.005679000  | -0.016511000 | 1.872565000  |

**II[Cl<sup>-</sup>] (B3LYP)**

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.707372000 | -2.318467000 | -0.184842000 |
| C | 2.891135000 | -3.628161000 | 0.318588000  |
| C | 1.661968000 | -4.279242000 | 0.269776000  |
| C | 0.711374000 | -3.376828000 | -0.269845000 |
| N | 1.401477000 | -2.242687000 | -0.582371000 |
| C | 4.745145000 | 0.689587000  | 0.296385000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 4.745124000  | -0.688760000 | 0.296337000  |
| C  | 3.431305000  | -1.088014000 | -0.151408000 |
| N  | 2.698956000  | 0.000468000  | -0.427190000 |
| C  | 3.431314000  | 1.088907000  | -0.151269000 |
| N  | 1.401459000  | 2.243595000  | -0.581936000 |
| C  | 0.711373000  | 3.377726000  | -0.269359000 |
| C  | 1.662011000  | 4.280140000  | 0.270199000  |
| C  | 2.891181000  | 3.629058000  | 0.318918000  |
| C  | 2.707380000  | 2.319365000  | -0.184519000 |
| C  | -0.712136000 | -3.376825000 | -0.269927000 |
| C  | -1.662727000 | -4.279136000 | 0.269870000  |
| C  | -2.891867000 | -3.628010000 | 0.318656000  |
| C  | -2.708123000 | -2.318436000 | -0.185087000 |
| N  | -1.402231000 | -2.242739000 | -0.582681000 |
| N  | -1.402217000 | 2.243650000  | -0.582248000 |
| C  | -2.708131000 | 2.319334000  | -0.184754000 |
| C  | -2.891907000 | 3.628899000  | 0.319019000  |
| C  | -1.662767000 | 4.280031000  | 0.270310000  |
| C  | -0.712136000 | 3.377724000  | -0.269438000 |
| N  | -2.699881000 | 0.000469000  | -0.427935000 |
| C  | -3.432096000 | -1.088015000 | -0.151811000 |
| C  | -4.745721000 | -0.688756000 | 0.296548000  |
| C  | -4.745729000 | 0.689578000  | 0.296639000  |
| C  | -3.432106000 | 1.088908000  | -0.151662000 |
| H  | 3.810077000  | -4.020041000 | 0.723945000  |
| H  | 1.444228000  | -5.271655000 | 0.630800000  |
| H  | 1.030882000  | -1.397078000 | -1.034901000 |
| H  | 5.560767000  | 1.336540000  | 0.584082000  |
| H  | 5.560732000  | -1.335757000 | 0.583975000  |
| H  | 1.030827000  | 1.397936000  | -1.034351000 |
| H  | 1.444308000  | 5.272565000  | 0.631215000  |
| H  | 3.810163000  | 4.020952000  | 0.724172000  |
| H  | -1.444960000 | -5.271465000 | 0.631108000  |
| H  | -3.810788000 | -4.019766000 | 0.724183000  |
| H  | -1.031655000 | -1.397268000 | -1.035494000 |
| H  | -1.031610000 | 1.398130000  | -1.034960000 |
| H  | -3.810862000 | 4.020662000  | 0.724462000  |
| H  | -1.445033000 | 5.272368000  | 0.631546000  |
| H  | -5.561187000 | -1.335750000 | 0.584594000  |
| H  | -5.561200000 | 1.336525000  | 0.584776000  |
| Cl | -0.000004000 | 0.000635000  | -2.483208000 |

**II[Cl<sup>-</sup>] (M06-2X)**

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 2.693957000 | -2.311947000 | -0.184391000 |
| C | 2.885426000 | -3.621768000 | 0.310276000  |
| C | 1.660195000 | -4.272391000 | 0.265153000  |
| C | 0.709974000 | -3.367230000 | -0.263679000 |
| N | 1.390361000 | -2.232782000 | -0.566457000 |
| C | 4.726680000 | 0.687005000  | 0.292586000  |
| C | 4.726635000 | -0.686188000 | 0.292624000  |
| C | 3.414254000 | -1.082183000 | -0.157391000 |
| N | 2.681939000 | 0.000456000  | -0.434172000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 3.414265000  | 1.083058000  | -0.157272000 |
| N  | 1.390289000  | 2.233663000  | -0.565852000 |
| C  | 0.709968000  | 3.368138000  | -0.263038000 |
| C  | 1.660296000  | 4.273316000  | 0.265564000  |
| C  | 2.885532000  | 3.622677000  | 0.310490000  |
| C  | 2.693953000  | 2.312822000  | -0.184046000 |
| C  | -0.710743000 | -3.367215000 | -0.263830000 |
| C  | -1.660996000 | -4.272306000 | 0.265037000  |
| C  | -2.886120000 | -3.621507000 | 0.310479000  |
| C  | -2.694715000 | -2.311895000 | -0.184750000 |
| N  | -1.391116000 | -2.232815000 | -0.566882000 |
| N  | -1.391077000 | 2.233720000  | -0.566282000 |
| C  | -2.694733000 | 2.312792000  | -0.184375000 |
| C  | -2.886228000 | 3.622430000  | 0.310752000  |
| C  | -1.661093000 | 4.273234000  | 0.265499000  |
| C  | -0.710751000 | 3.368133000  | -0.263183000 |
| N  | -2.682961000 | 0.000470000  | -0.435328000 |
| C  | -3.415083000 | -1.082174000 | -0.158029000 |
| C  | -4.727171000 | -0.686189000 | 0.292845000  |
| C  | -4.727224000 | 0.686998000  | 0.292820000  |
| C  | -3.415107000 | 1.083065000  | -0.157889000 |
| H  | 3.810446000  | -4.011140000 | 0.703698000  |
| H  | 1.440394000  | -5.267332000 | 0.617342000  |
| H  | 1.019208000  | -1.380045000 | -1.004073000 |
| H  | 5.537215000  | 1.338326000  | 0.582289000  |
| H  | 5.537140000  | -1.337545000 | 0.582331000  |
| H  | 1.018938000  | 1.380799000  | -1.003020000 |
| H  | 1.440593000  | 5.268312000  | 0.617659000  |
| H  | 3.810650000  | 4.012086000  | 0.703644000  |
| H  | -1.441197000 | -5.267196000 | 0.617372000  |
| H  | -3.811071000 | -4.010709000 | 0.704228000  |
| H  | -1.020062000 | -1.380157000 | -1.004792000 |
| H  | -1.019865000 | 1.380934000  | -1.003773000 |
| H  | -3.811265000 | 4.011671000  | 0.704262000  |
| H  | -1.441375000 | 5.268167000  | 0.617764000  |
| H  | -5.537439000 | -1.337570000 | 0.583161000  |
| H  | -5.537532000 | 1.338327000  | 0.583140000  |
| Cl | 0.000100000  | 0.000581000  | -2.449604000 |

### III[Cl] (B3LYP)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 2.153747000  | 0.108801000  | 1.412526000  |
| C | 1.262796000  | 1.160575000  | 1.475915000  |
| C | 1.669412000  | 2.150708000  | 0.550611000  |
| N | 2.878510000  | 1.729638000  | 0.013961000  |
| C | 3.138450000  | 0.420116000  | 0.437475000  |
| C | 4.085552000  | -1.780951000 | -0.198440000 |
| C | 5.082611000  | -2.687020000 | -0.690024000 |
| C | 4.527232000  | -3.946110000 | -0.761320000 |
| C | 3.162333000  | -3.850911000 | -0.340169000 |
| N | 2.963935000  | -2.542762000 | 0.039077000  |
| C | -3.176238000 | -0.383105000 | 0.413749000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -2.187082000 | -0.060297000 | 1.377848000  |
| C  | -1.294025000 | -1.112356000 | 1.480509000  |
| C  | -1.710621000 | -2.111698000 | 0.569338000  |
| N  | -2.915706000 | -1.695075000 | 0.016306000  |
| N  | -0.402351000 | 3.325583000  | 0.258332000  |
| C  | -0.814611000 | 4.515294000  | -0.267113000 |
| C  | 0.329990000  | 5.296544000  | -0.698296000 |
| C  | 1.435580000  | 4.516138000  | -0.477923000 |
| C  | 0.948369000  | 3.298442000  | 0.136130000  |
| N  | -3.009841000 | 2.575052000  | -0.001122000 |
| C  | -4.130445000 | 1.808764000  | -0.240637000 |
| C  | -5.130218000 | 2.716619000  | -0.728492000 |
| C  | -4.577281000 | 3.975600000  | -0.801322000 |
| C  | -3.209467000 | 3.885050000  | -0.383574000 |
| C  | -0.379929000 | -5.281300000 | -0.635837000 |
| C  | -1.483350000 | -4.500614000 | -0.418596000 |
| C  | -0.990334000 | -3.265713000 | 0.165933000  |
| N  | 0.356762000  | -3.284398000 | 0.266817000  |
| C  | 0.768681000  | -4.485459000 | -0.233553000 |
| C  | 2.123853000  | -4.785426000 | -0.450965000 |
| C  | 4.151190000  | -0.383395000 | -0.104662000 |
| C  | -4.196719000 | 0.415420000  | -0.132708000 |
| C  | -2.173609000 | 4.817044000  | -0.490193000 |
| H  | 2.124227000  | -0.738731000 | 2.088793000  |
| H  | 0.451235000  | 1.239212000  | 2.182020000  |
| H  | 3.217104000  | 2.080813000  | -0.869483000 |
| H  | 6.090923000  | -2.397777000 | -0.955424000 |
| H  | 5.001968000  | -4.853991000 | -1.109356000 |
| H  | -2.184605000 | 0.834167000  | 1.984052000  |
| H  | -0.488773000 | -1.200328000 | 2.212726000  |
| H  | -3.263882000 | -2.069666000 | -0.853491000 |
| H  | 0.296801000  | 6.291157000  | -1.127162000 |
| H  | 2.472272000  | 4.770977000  | -0.663002000 |
| H  | -6.139202000 | 2.426809000  | -0.991032000 |
| H  | -5.055606000 | 4.882407000  | -1.147570000 |
| H  | -0.348582000 | -6.286657000 | -1.038881000 |
| H  | -2.521732000 | -4.762785000 | -0.582959000 |
| H  | 2.382348000  | -5.766420000 | -0.838478000 |
| H  | 5.000086000  | 0.092661000  | -0.590192000 |
| H  | -5.054290000 | -0.066971000 | -0.595503000 |
| H  | -2.427391000 | 5.795876000  | -0.886213000 |
| H  | -2.058250000 | 2.269926000  | 0.224282000  |
| H  | 2.019216000  | -2.240077000 | 0.297313000  |
| Cl | 0.645902000  | -0.854579000 | 4.299975000  |

### III[Cl<sup>-</sup>] (M06-2X)

|   |             |             |              |
|---|-------------|-------------|--------------|
| C | 2.196690000 | 0.039721000 | 1.360781000  |
| C | 1.271778000 | 1.084146000 | 1.425183000  |
| C | 1.671689000 | 2.045602000 | 0.498002000  |
| N | 2.861614000 | 1.623225000 | -0.065602000 |
| C | 3.162593000 | 0.357426000 | 0.397502000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 4.142371000  | -1.807291000 | -0.211687000 |
| C  | 5.141482000  | -2.746744000 | -0.686750000 |
| C  | 4.579952000  | -3.981597000 | -0.744213000 |
| C  | 3.193638000  | -3.871446000 | -0.333163000 |
| N  | 3.015467000  | -2.560002000 | 0.040149000  |
| C  | -3.119032000 | -0.399140000 | 0.384478000  |
| C  | -2.072461000 | -0.032303000 | 1.303012000  |
| C  | -1.190797000 | -1.065919000 | 1.381175000  |
| C  | -1.648008000 | -2.114951000 | 0.518061000  |
| N  | -2.879650000 | -1.734019000 | 0.036010000  |
| N  | -0.378908000 | 3.222183000  | 0.182287000  |
| C  | -0.792829000 | 4.461215000  | -0.251535000 |
| C  | 0.363290000  | 5.270453000  | -0.604681000 |
| C  | 1.452933000  | 4.478296000  | -0.416035000 |
| C  | 0.943199000  | 3.212282000  | 0.099458000  |
| N  | -2.966787000 | 2.518678000  | -0.017194000 |
| C  | -4.100308000 | 1.785379000  | -0.196526000 |
| C  | -5.112032000 | 2.691615000  | -0.596385000 |
| C  | -4.548165000 | 3.957627000  | -0.659371000 |
| C  | -3.181698000 | 3.836536000  | -0.317493000 |
| C  | -0.326694000 | -5.238647000 | -0.707355000 |
| C  | -1.430706000 | -4.460207000 | -0.500345000 |
| C  | -0.949964000 | -3.265112000 | 0.146229000  |
| N  | 0.406818000  | -3.312097000 | 0.309507000  |
| C  | 0.807415000  | -4.472497000 | -0.226905000 |
| C  | 2.183268000  | -4.798062000 | -0.431796000 |
| C  | 4.232762000  | -0.442080000 | -0.111820000 |
| C  | -4.135168000 | 0.363190000  | -0.136902000 |
| C  | -2.125665000 | 4.772607000  | -0.433971000 |
| H  | 2.211785000  | -0.838444000 | 1.992342000  |
| H  | 0.456102000  | 1.178697000  | 2.141856000  |
| H  | 3.241841000  | 2.004310000  | -0.917667000 |
| H  | 6.152614000  | -2.467445000 | -0.951164000 |
| H  | 5.041221000  | -4.901847000 | -1.077018000 |
| H  | -2.030722000 | 0.844706000  | 1.942058000  |
| H  | -0.353331000 | -1.124703000 | 2.060791000  |
| H  | -3.264814000 | -2.141175000 | -0.802323000 |
| H  | 0.334873000  | 6.294148000  | -0.956071000 |
| H  | 2.495456000  | 4.733219000  | -0.557645000 |
| H  | -6.135560000 | 2.415866000  | -0.808301000 |
| H  | -5.035085000 | 4.880119000  | -0.944005000 |
| H  | -0.281030000 | -6.222970000 | -1.156246000 |
| H  | -2.463648000 | -4.700890000 | -0.719693000 |
| H  | 2.435152000  | -5.783310000 | -0.809946000 |
| H  | 5.131292000  | 0.033992000  | -0.493479000 |
| H  | -4.960919000 | -0.123532000 | -0.649202000 |
| H  | -2.389755000 | 5.769501000  | -0.775063000 |
| H  | -2.017220000 | 2.196341000  | 0.195215000  |
| H  | 2.080357000  | -2.218118000 | 0.263152000  |
| Cl | -0.714559000 | 0.748492000  | 4.190300000  |

IV[Cl<sup>-</sup>] (B3LYP)

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 2.193784000  | 0.064390000  | -0.234621000 |
| C  | 2.908506000  | -1.062571000 | 0.039934000  |
| C  | 4.174121000  | -0.646518000 | 0.478632000  |
| C  | 4.175955000  | 0.770881000  | 0.478081000  |
| C  | 2.911517000  | 1.189579000  | 0.038738000  |
| C  | 1.444497000  | -4.458360000 | -0.024415000 |
| C  | 2.589602000  | -3.709949000 | 0.002798000  |
| C  | 2.160590000  | -2.312435000 | -0.008866000 |
| N  | 0.843152000  | -2.219921000 | -0.032357000 |
| C  | 0.338544000  | -3.510214000 | -0.052217000 |
| N  | 0.847328000  | 2.345900000  | -0.028990000 |
| C  | 2.164300000  | 2.440357000  | -0.013156000 |
| C  | 2.592315000  | 3.838462000  | -0.015499000 |
| C  | 1.446294000  | 4.585352000  | -0.043160000 |
| C  | 0.341262000  | 3.635422000  | -0.059124000 |
| C  | -2.036359000 | 2.857792000  | -0.037799000 |
| C  | -3.399844000 | 2.979190000  | 0.303400000  |
| C  | -3.953085000 | 1.692290000  | 0.326226000  |
| C  | -2.930272000 | 0.788457000  | -0.025058000 |
| N  | -1.799661000 | 1.515867000  | -0.241979000 |
| C  | -2.931245000 | -0.664095000 | -0.028820000 |
| C  | -3.961992000 | -1.569694000 | 0.294589000  |
| C  | -3.409826000 | -2.857060000 | 0.276098000  |
| C  | -2.039521000 | -2.735434000 | -0.036750000 |
| N  | -1.798013000 | -1.392420000 | -0.226245000 |
| C  | -1.018481000 | 3.861971000  | -0.052877000 |
| C  | -1.021236000 | -3.738563000 | -0.045595000 |
| H  | 1.299440000  | 0.067074000  | -0.745056000 |
| H  | 4.975889000  | -1.292632000 | 0.810972000  |
| H  | 4.979508000  | 1.415198000  | 0.809559000  |
| H  | 1.362122000  | -5.538894000 | -0.035354000 |
| H  | 3.611912000  | -4.067315000 | 0.024318000  |
| H  | 3.614319000  | 4.197181000  | -0.001871000 |
| H  | 1.362684000  | 5.665665000  | -0.063618000 |
| H  | -3.899098000 | 3.906546000  | 0.552366000  |
| H  | -4.965674000 | 1.421961000  | 0.591527000  |
| H  | -0.949705000 | 1.164724000  | -0.711075000 |
| H  | -4.980850000 | -1.300144000 | 0.535459000  |
| H  | -3.916143000 | -3.785701000 | 0.505048000  |
| H  | -0.928105000 | -1.043855000 | -0.652456000 |
| H  | -1.369939000 | 4.890279000  | 0.000280000  |
| H  | -1.371716000 | -4.767000000 | 0.009866000  |
| Cl | -0.107656000 | 0.079316000  | -2.492404000 |

**IV[Cl<sup>-</sup>] (M06-2X)**

|   |             |              |              |
|---|-------------|--------------|--------------|
| N | 2.181817000 | 0.062422000  | -0.206659000 |
| C | 2.898122000 | -1.055858000 | 0.058659000  |
| C | 4.159634000 | -0.645670000 | 0.491291000  |
| C | 4.159833000 | 0.770581000  | 0.490645000  |
| C | 2.898423000 | 1.180735000  | 0.057675000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 1.441696000  | -4.447024000 | -0.061575000 |
| C  | 2.578655000  | -3.702044000 | -0.023028000 |
| C  | 2.143037000  | -2.304689000 | -0.006428000 |
| N  | 0.838466000  | -2.208643000 | -0.024096000 |
| C  | 0.333681000  | -3.499156000 | -0.067566000 |
| N  | 0.839057000  | 2.333980000  | -0.025446000 |
| C  | 2.143647000  | 2.429714000  | -0.008389000 |
| C  | 2.579635000  | 3.826947000  | -0.026905000 |
| C  | 1.442865000  | 4.572171000  | -0.065895000 |
| C  | 0.334591000  | 3.624570000  | -0.070400000 |
| C  | -2.031810000 | 2.847781000  | -0.032377000 |
| C  | -3.391766000 | 2.975246000  | 0.285651000  |
| C  | -3.944705000 | 1.688962000  | 0.312100000  |
| C  | -2.918123000 | 0.791494000  | -0.011695000 |
| N  | -1.789592000 | 1.510778000  | -0.212872000 |
| C  | -2.918281000 | -0.665108000 | -0.011142000 |
| C  | -3.945113000 | -1.562091000 | 0.313255000  |
| C  | -3.392497000 | -2.848518000 | 0.287855000  |
| C  | -2.032492000 | -2.721645000 | -0.030252000 |
| N  | -1.789928000 | -1.384837000 | -0.211700000 |
| C  | -1.013557000 | 3.855582000  | -0.062973000 |
| C  | -1.014548000 | -3.729758000 | -0.059840000 |
| H  | 1.278325000  | 0.062280000  | -0.702140000 |
| H  | 4.962648000  | -1.293290000 | 0.814467000  |
| H  | 4.963029000  | 1.418268000  | 0.813233000  |
| H  | 1.354755000  | -5.525838000 | -0.093073000 |
| H  | 3.603090000  | -4.050513000 | -0.012739000 |
| H  | 3.604172000  | 4.175142000  | -0.017463000 |
| H  | 1.356181000  | 5.650969000  | -0.098707000 |
| H  | -3.893561000 | 3.907211000  | 0.507741000  |
| H  | -4.961368000 | 1.416536000  | 0.556169000  |
| H  | -0.919498000 | 1.156443000  | -0.633272000 |
| H  | -4.961731000 | -1.289202000 | 0.556987000  |
| H  | -3.894528000 | -3.780205000 | 0.510570000  |
| H  | -0.919474000 | -1.031050000 | -0.631724000 |
| H  | -1.364812000 | 4.884766000  | -0.030092000 |
| H  | -1.366139000 | -4.758788000 | -0.025771000 |
| Cl | -0.082618000 | 0.062427000  | -2.423551000 |

### V[Cl] (B3LYP)

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 3.666853000 | 1.165988000  | 0.039868000  |
| C | 4.791860000 | 2.092658000  | -0.093645000 |
| C | 4.244628000 | 3.339436000  | -0.092658000 |
| C | 2.809247000 | 3.143424000  | 0.028706000  |
| N | 2.507422000 | 1.794327000  | 0.123551000  |
| C | 4.725937000 | -2.331151000 | 0.204040000  |
| C | 5.031197000 | -0.976177000 | 0.226254000  |
| C | 3.817048000 | -0.273437000 | 0.085670000  |
| N | 2.799517000 | -1.178781000 | -0.005107000 |
| C | 3.326774000 | -2.457520000 | 0.061431000  |
| N | 0.301584000 | -3.081551000 | 0.123302000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -0.822408000 | -3.771496000 | 0.041599000  |
| C  | -0.582534000 | -5.208850000 | -0.094778000 |
| C  | 0.770849000  | -5.358128000 | -0.097619000 |
| C  | 1.318939000  | -4.017090000 | 0.024328000  |
| C  | 0.455074000  | 4.103386000  | 0.066080000  |
| C  | -0.353807000 | 5.251950000  | 0.209480000  |
| C  | -1.680133000 | 4.839354000  | 0.227707000  |
| C  | -1.681874000 | 3.436868000  | 0.084195000  |
| N  | -0.389081000 | 3.007970000  | -0.004632000 |
| N  | -2.418956000 | -1.847813000 | -0.000759000 |
| C  | -3.789849000 | -1.664343000 | 0.067109000  |
| C  | -4.380355000 | -2.938926000 | 0.211121000  |
| C  | -3.359837000 | -3.881178000 | 0.232477000  |
| C  | -2.144020000 | -3.181689000 | 0.090157000  |
| N  | -2.816745000 | 1.268871000  | 0.120661000  |
| C  | -2.853117000 | 2.586945000  | 0.035621000  |
| C  | -4.218152000 | 3.096912000  | -0.101222000 |
| C  | -5.023506000 | 1.999044000  | -0.100609000 |
| C  | -4.135526000 | 0.854614000  | 0.023844000  |
| H  | 5.836496000  | 1.826041000  | -0.190240000 |
| H  | 4.750504000  | 4.292814000  | -0.188674000 |
| H  | 5.408778000  | -3.165282000 | 0.299882000  |
| H  | 6.004170000  | -0.521603000 | 0.344375000  |
| H  | -1.335970000 | -5.980133000 | -0.190383000 |
| H  | 1.343400000  | -6.272709000 | -0.196498000 |
| H  | 0.027275000  | 6.260064000  | 0.308022000  |
| H  | -2.560357000 | 5.454589000  | 0.345479000  |
| H  | -0.118440000 | 2.031254000  | -0.249942000 |
| H  | -1.708541000 | -1.125332000 | -0.246946000 |
| H  | -5.444112000 | -3.113034000 | 0.307858000  |
| H  | -3.453131000 | -4.950997000 | 0.350879000  |
| H  | -4.509955000 | 4.134655000  | -0.199450000 |
| H  | -6.101905000 | 1.959638000  | -0.198428000 |
| C  | 2.657705000  | -3.704882000 | 0.019590000  |
| H  | 3.339994000  | -4.552722000 | -0.014558000 |
| H  | 1.818104000  | -0.924974000 | -0.250050000 |
| C  | -4.534795000 | -0.460881000 | 0.023235000  |
| H  | -5.610308000 | -0.627193000 | -0.009533000 |
| C  | 1.869878000  | 4.147129000  | 0.026162000  |
| H  | 2.263297000  | 5.161882000  | -0.004708000 |
| Cl | -0.004238000 | -0.007185000 | -1.271612000 |

**V[Cl<sup>-</sup>] (M06-2X)**

|   |             |              |              |
|---|-------------|--------------|--------------|
| C | 3.615943000 | 1.161076000  | 0.040669000  |
| C | 4.756947000 | 2.072589000  | -0.104616000 |
| C | 4.229226000 | 3.318102000  | -0.107818000 |
| C | 2.790670000 | 3.138915000  | 0.020980000  |
| N | 2.472877000 | 1.790901000  | 0.123348000  |
| C | 4.706453000 | -2.317640000 | 0.230665000  |
| C | 4.995197000 | -0.957462000 | 0.249728000  |
| C | 3.778250000 | -0.280302000 | 0.099024000  |



|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 2.776249000  | -1.192050000 | 0.005516000  |
| C  | 3.319099000  | -2.453172000 | 0.078782000  |
| N  | 0.319437000  | -3.051188000 | 0.123157000  |
| C  | -0.798355000 | -3.722942000 | 0.028214000  |
| C  | -0.581815000 | -5.164946000 | -0.135547000 |
| C  | 0.760283000  | -5.333604000 | -0.135788000 |
| C  | 1.326520000  | -4.001010000 | 0.011673000  |
| C  | 0.453214000  | 4.092001000  | 0.068663000  |
| C  | -0.357338000 | 5.227584000  | 0.208046000  |
| C  | -1.680219000 | 4.799048000  | 0.222191000  |
| C  | -1.658503000 | 3.405594000  | 0.081514000  |
| N  | -0.367912000 | 2.991465000  | -0.001333000 |
| N  | -2.415983000 | -1.818459000 | 0.006257000  |
| C  | -3.779418000 | -1.658600000 | 0.087007000  |
| C  | -4.354987000 | -2.928547000 | 0.236838000  |
| C  | -3.321324000 | -3.858524000 | 0.246255000  |
| C  | -2.127355000 | -3.142239000 | 0.092835000  |
| N  | -2.799322000 | 1.240764000  | 0.121421000  |
| C  | -2.825942000 | 2.544766000  | 0.029185000  |
| C  | -4.186156000 | 3.075800000  | -0.116174000 |
| C  | -5.000927000 | 1.996279000  | -0.108168000 |
| C  | -4.125890000 | 0.840985000  | 0.026197000  |
| H  | 5.794861000  | 1.785689000  | -0.205874000 |
| H  | 4.738971000  | 4.267699000  | -0.211142000 |
| H  | 5.395965000  | -3.145240000 | 0.328164000  |
| H  | 5.960665000  | -0.489051000 | 0.371261000  |
| H  | -1.350694000 | -5.916921000 | -0.251036000 |
| H  | 1.325436000  | -6.250173000 | -0.248738000 |
| H  | 0.016244000  | 6.238377000  | 0.300821000  |
| H  | -2.569409000 | 5.401696000  | 0.333132000  |
| H  | -0.081471000 | 2.013671000  | -0.222363000 |
| H  | -1.714252000 | -1.082292000 | -0.224443000 |
| H  | -5.416011000 | -3.111896000 | 0.339551000  |
| H  | -3.396382000 | -4.929414000 | 0.364172000  |
| H  | -4.456486000 | 4.117493000  | -0.224322000 |
| H  | -6.078544000 | 1.962734000  | -0.207524000 |
| C  | 2.656062000  | -3.710005000 | 0.015515000  |
| H  | 3.337361000  | -4.557944000 | -0.032483000 |
| H  | 1.788192000  | -0.951434000 | -0.222579000 |
| C  | -4.537176000 | -0.456369000 | 0.032712000  |
| H  | -5.612449000 | -0.623111000 | -0.005130000 |
| C  | 1.873379000  | 4.144694000  | 0.017021000  |
| H  | 2.268018000  | 5.158501000  | -0.027343000 |
| Cl | -0.006321000 | -0.007130000 | -1.197457000 |

#### VI[Cl<sup>-</sup>] (B3LYP)

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 0.934055000  | 4.522183000 | -0.442589000 |
| C | -0.468192000 | 4.633324000 | -0.471648000 |
| C | -0.994189000 | 3.381283000 | -0.132796000 |
| N | 0.060035000  | 2.535237000 | 0.094213000  |
| C | 1.244033000  | 3.203976000 | -0.078375000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 2.544168000  | 2.583379000  | 0.029820000  |
| C  | 3.807285000  | 3.210150000  | -0.030862000 |
| C  | 4.778232000  | 2.211271000  | 0.040807000  |
| C  | 4.117943000  | 0.969675000  | 0.135412000  |
| N  | 2.759526000  | 1.240051000  | 0.134448000  |
| C  | -1.248900000 | -3.210518000 | -0.080141000 |
| C  | -0.939305000 | -4.528442000 | -0.445672000 |
| C  | 0.462914000  | -4.639558000 | -0.476379000 |
| C  | 0.989261000  | -3.387753000 | -0.137187000 |
| N  | -0.064706000 | -2.541890000 | 0.091649000  |
| N  | -2.643878000 | 1.614394000  | 0.008391000  |
| C  | -4.027018000 | 1.526519000  | 0.090487000  |
| C  | -4.610875000 | 2.854696000  | 0.071681000  |
| C  | -3.564201000 | 3.728496000  | -0.017855000 |
| C  | -2.359313000 | 2.908385000  | -0.047269000 |
| N  | -2.764172000 | -1.246791000 | 0.136412000  |
| C  | -2.548915000 | -2.590001000 | 0.029913000  |
| C  | -3.812103000 | -3.216679000 | -0.030327000 |
| C  | -4.782965000 | -2.217874000 | 0.043428000  |
| C  | -4.122566000 | -0.976392000 | 0.138859000  |
| C  | 4.606152000  | -2.861322000 | 0.063852000  |
| C  | 3.559381000  | -3.735039000 | -0.025293000 |
| C  | 2.354465000  | -2.914904000 | -0.052713000 |
| N  | 2.639082000  | -1.620962000 | 0.003910000  |
| C  | 4.022308000  | -1.533176000 | 0.084687000  |
| C  | 4.687937000  | -0.326173000 | 0.146713000  |
| C  | -4.692571000 | 0.319446000  | 0.151974000  |
| H  | 1.653001000  | 5.290732000  | -0.691113000 |
| H  | -1.045821000 | 5.506531000  | -0.742745000 |
| H  | -0.044636000 | 1.614047000  | 0.565427000  |
| H  | 3.966569000  | 4.275467000  | -0.116799000 |
| H  | 5.852407000  | 2.338611000  | 0.010363000  |
| H  | -1.658521000 | -5.296823000 | -0.693939000 |
| H  | 1.040255000  | -5.512570000 | -0.748702000 |
| H  | 0.040487000  | -1.621153000 | 0.563679000  |
| H  | -5.668179000 | 3.085604000  | 0.126178000  |
| H  | -3.600453000 | 4.810303000  | -0.046310000 |
| H  | -3.971479000 | -4.281892000 | -0.117390000 |
| H  | -5.857170000 | -2.345137000 | 0.013776000  |
| H  | 5.663518000  | -3.092269000 | 0.116954000  |
| H  | 3.595589000  | -4.816820000 | -0.054774000 |
| H  | 5.775034000  | -0.352710000 | 0.177317000  |
| H  | -5.779637000 | 0.345945000  | 0.183686000  |
| H  | -2.066726000 | -0.511502000 | 0.281817000  |
| H  | 2.062290000  | 0.504475000  | 0.279437000  |
| Cl | -0.001417000 | -0.004422000 | 1.865587000  |

**VI[Cl<sup>-</sup>] (M06-2X)**

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | 0.930824000  | 4.522106000 | -0.465322000 |
| C | -0.471865000 | 4.638203000 | -0.494487000 |
| C | -0.992118000 | 3.390956000 | -0.163088000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| N  | 0.052607000  | 2.544875000  | 0.059114000  |
| C  | 1.229067000  | 3.207791000  | -0.106496000 |
| C  | 2.528360000  | 2.577492000  | 0.020823000  |
| C  | 3.784593000  | 3.197100000  | -0.028841000 |
| C  | 4.746881000  | 2.190876000  | 0.064101000  |
| C  | 4.076104000  | 0.965309000  | 0.160890000  |
| N  | 2.725957000  | 1.239386000  | 0.138085000  |
| C  | -1.233986000 | -3.214309000 | -0.108427000 |
| C  | -0.936095000 | -4.528352000 | -0.468534000 |
| C  | 0.466565000  | -4.644359000 | -0.499380000 |
| C  | 0.987142000  | -3.397359000 | -0.167556000 |
| N  | -0.057368000 | -2.551476000 | 0.056398000  |
| N  | -2.618476000 | 1.620604000  | 0.010541000  |
| C  | -3.999937000 | 1.523389000  | 0.118458000  |
| C  | -4.593875000 | 2.849792000  | 0.102346000  |
| C  | -3.560837000 | 3.723352000  | -0.012617000 |
| C  | -2.352850000 | 2.904209000  | -0.058886000 |
| N  | -2.730585000 | -1.246144000 | 0.139755000  |
| C  | -2.533136000 | -2.584130000 | 0.020851000  |
| C  | -3.789431000 | -3.203662000 | -0.028141000 |
| C  | -4.751606000 | -2.197513000 | 0.066826000  |
| C  | -4.080707000 | -0.972065000 | 0.164253000  |
| C  | 4.589172000  | -2.856490000 | 0.094700000  |
| C  | 3.555996000  | -3.729925000 | -0.019951000 |
| C  | 2.347984000  | -2.910712000 | -0.064327000 |
| N  | 2.613711000  | -1.627178000 | 0.005967000  |
| C  | 3.995280000  | -1.530090000 | 0.112615000  |
| C  | 4.651739000  | -0.333262000 | 0.187529000  |
| C  | -4.656309000 | 0.326479000  | 0.192818000  |
| H  | 1.656116000  | 5.287845000  | -0.701215000 |
| H  | -1.050223000 | 5.513389000  | -0.755442000 |
| H  | -0.060945000 | 1.610194000  | 0.496725000  |
| H  | 3.947021000  | 4.260716000  | -0.122486000 |
| H  | 5.822313000  | 2.304534000  | 0.046868000  |
| H  | -1.661617000 | -5.293961000 | -0.704143000 |
| H  | 1.044677000  | -5.519338000 | -0.761575000 |
| H  | 0.056628000  | -1.617178000 | 0.494726000  |
| H  | -5.651995000 | 3.067632000  | 0.175006000  |
| H  | -3.594734000 | 4.804192000  | -0.049028000 |
| H  | -3.951980000 | -4.267174000 | -0.122757000 |
| H  | -5.827056000 | -2.311133000 | 0.050559000  |
| H  | 5.647359000  | -3.074421000 | 0.166097000  |
| H  | 3.589832000  | -4.810736000 | -0.057321000 |
| H  | 5.738259000  | -0.354531000 | 0.240195000  |
| H  | -5.742778000 | 0.347688000  | 0.246573000  |
| H  | -2.017681000 | -0.524565000 | 0.286657000  |
| H  | 2.013210000  | 0.517647000  | 0.284983000  |
| Cl | -0.001191000 | -0.004283000 | 1.755559000  |

**VII (B3LYP)**

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -0.594606000 | 4.367478000 | -0.012378000 |
| H | -0.323815000 | 3.459693000 | 0.518581000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.482460000  | 5.321830000  | -0.126563000 |
| C | 1.832795000  | 5.024120000  | 0.099631000  |
| C | 2.289789000  | 3.679821000  | 0.198400000  |
| H | 1.576615000  | 2.881262000  | 0.017219000  |
| C | 3.616096000  | 3.314040000  | 0.413451000  |
| C | 4.652552000  | 4.375965000  | 0.715732000  |
| H | 5.325348000  | 4.031517000  | 1.504009000  |
| C | 4.012192000  | 5.706482000  | 1.126571000  |
| C | 2.884733000  | 6.111996000  | 0.171494000  |
| H | 3.294007000  | 6.280667000  | -0.835164000 |
| C | 3.902354000  | 1.927262000  | 0.292917000  |
| H | 3.027202000  | 1.314467000  | 0.100848000  |
| C | 5.113949000  | 1.234832000  | 0.342460000  |
| C | 6.349880000  | 1.933143000  | 0.558824000  |
| N | 7.379229000  | 2.449601000  | 0.728108000  |
| C | 5.231355000  | -0.196893000 | 0.163319000  |
| C | 4.130026000  | -1.034305000 | -0.018338000 |
| H | 3.133946000  | -0.605183000 | -0.047023000 |
| C | 4.204403000  | -2.441111000 | -0.103545000 |
| C | 5.559714000  | -3.104250000 | -0.092082000 |
| H | 5.760800000  | -3.467242000 | 0.926967000  |
| C | 6.665820000  | -2.146388000 | -0.541148000 |
| C | 6.607281000  | -0.819052000 | 0.213120000  |
| C | 2.972836000  | -3.132359000 | -0.178853000 |
| H | 2.104779000  | -2.484840000 | -0.246836000 |
| C | 2.691135000  | -4.501560000 | -0.185779000 |
| C | 3.750768000  | -5.467040000 | -0.077946000 |
| N | 4.565199000  | -6.291379000 | 0.030269000  |
| C | 1.366578000  | -5.075371000 | -0.270229000 |
| C | 0.229173000  | -4.300387000 | -0.130190000 |
| H | 0.331166000  | -3.235330000 | 0.056228000  |
| C | -1.107879000 | -4.804726000 | -0.138920000 |
| C | -1.315592000 | -6.283411000 | -0.392537000 |
| H | -1.449873000 | -6.795555000 | 0.569717000  |
| C | -0.129946000 | -6.897014000 | -1.146466000 |
| C | 1.206786000  | -6.570762000 | -0.472884000 |
| H | 2.033475000  | -6.964396000 | -1.070282000 |
| C | -2.103515000 | -3.877393000 | 0.110619000  |
| H | -1.755338000 | -2.857868000 | 0.240637000  |
| C | -3.521241000 | -4.044028000 | 0.279376000  |
| C | -4.071889000 | -5.363162000 | 0.410198000  |
| N | -4.543646000 | -6.420152000 | 0.534609000  |
| C | -4.414240000 | -2.971483000 | 0.392673000  |
| C | -4.011735000 | -1.610667000 | 0.179503000  |
| H | -3.007005000 | -1.417195000 | -0.180401000 |
| C | -4.842560000 | -0.524181000 | 0.333512000  |
| C | -6.250576000 | -0.698615000 | 0.849733000  |
| H | -6.499741000 | 0.108425000  | 1.543067000  |
| C | -6.452561000 | -2.055868000 | 1.531417000  |
| C | -5.876116000 | -3.202336000 | 0.692904000  |
| H | -6.416151000 | -3.267127000 | -0.264110000 |
| C | -4.285586000 | 0.763724000  | -0.023390000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -3.243960000 | 0.729761000  | -0.331488000 |
| C | -4.857402000 | 2.008554000  | -0.066395000 |
| C | -6.257318000 | 2.215607000  | 0.170537000  |
| N | -7.386874000 | 2.440422000  | 0.341439000  |
| C | -4.079076000 | 3.223196000  | -0.407757000 |
| C | -2.761977000 | 3.318238000  | -0.069601000 |
| H | -2.310319000 | 2.527398000  | 0.524327000  |
| C | -1.905669000 | 4.433727000  | -0.424717000 |
| C | -2.531501000 | 5.519117000  | -1.270253000 |
| H | -2.020826000 | 6.472453000  | -1.151516000 |
| C | -4.027005000 | 5.679840000  | -0.969121000 |
| C | -4.777098000 | 4.355571000  | -1.126610000 |
| H | -5.805011000 | 4.451701000  | -0.763660000 |
| C | 0.194437000  | 6.699752000  | -0.409521000 |
| N | 0.011840000  | 7.829587000  | -0.623890000 |
| H | 7.352612000  | -0.122031000 | -0.177677000 |
| H | 4.776939000  | 6.487349000  | 1.152960000  |
| H | 3.609618000  | 5.621196000  | 2.142953000  |
| H | -4.456986000 | 6.434482000  | -1.633279000 |
| H | -4.152210000 | 6.048105000  | 0.055777000  |
| H | -5.964596000 | -2.047453000 | 2.513220000  |
| H | -7.517941000 | -2.226161000 | 1.707959000  |
| H | -0.257088000 | -7.981114000 | -1.209822000 |
| H | -0.115464000 | -6.517366000 | -2.175213000 |
| H | 7.642014000  | -2.615623000 | -0.393716000 |
| H | 6.563667000  | -1.954152000 | -1.615672000 |
| H | 2.440836000  | 7.059383000  | 0.484058000  |
| H | 5.284991000  | 4.520108000  | -0.170473000 |
| H | 6.872397000  | -0.968029000 | 1.271907000  |
| H | 5.559314000  | -3.992023000 | -0.725084000 |
| H | 1.271489000  | -7.076870000 | 0.501105000  |
| H | -6.949845000 | -0.585881000 | 0.008977000  |
| H | -6.023415000 | -4.162347000 | 1.191882000  |
| H | -2.237968000 | -6.451517000 | -0.950606000 |
| H | -2.401638000 | 5.229847000  | -2.324601000 |
| H | -4.863583000 | 4.089167000  | -2.191410000 |

## VII (M06-2X)

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -0.596835000 | 4.365659000 | 0.142298000  |
| H | -0.342986000 | 3.503013000 | 0.752355000  |
| C | 0.480227000  | 5.333838000 | -0.004096000 |
| C | 1.818640000  | 5.043500000 | 0.142358000  |
| C | 2.268029000  | 3.681470000 | 0.221939000  |
| H | 1.538268000  | 2.894086000 | 0.052956000  |
| C | 3.584004000  | 3.319661000 | 0.398035000  |
| C | 4.639536000  | 4.362505000 | 0.683103000  |
| H | 5.309767000  | 4.006144000 | 1.468835000  |
| C | 4.017812000  | 5.694835000 | 1.099920000  |
| C | 2.890430000  | 6.105624000 | 0.153484000  |
| H | 3.286258000  | 6.221803000 | -0.864610000 |
| C | 3.858122000  | 1.924058000 | 0.261667000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 2.971020000  | 1.312354000  | 0.124196000  |
| C | 5.063057000  | 1.248436000  | 0.256064000  |
| C | 6.307037000  | 1.955030000  | 0.426143000  |
| N | 7.337341000  | 2.467739000  | 0.551660000  |
| C | 5.181533000  | -0.184159000 | 0.079221000  |
| C | 4.086403000  | -1.007464000 | -0.145881000 |
| H | 3.097709000  | -0.574908000 | -0.252978000 |
| C | 4.160386000  | -2.413740000 | -0.162447000 |
| C | 5.503253000  | -3.082402000 | -0.064045000 |
| H | 5.657795000  | -3.398391000 | 0.978449000  |
| C | 6.622490000  | -2.150400000 | -0.517038000 |
| C | 6.548989000  | -0.802948000 | 0.186314000  |
| C | 2.929549000  | -3.101144000 | -0.257993000 |
| H | 2.067353000  | -2.465779000 | -0.433625000 |
| C | 2.659288000  | -4.458871000 | -0.162496000 |
| C | 3.719195000  | -5.411340000 | 0.063488000  |
| N | 4.524060000  | -6.218782000 | 0.264101000  |
| C | 1.347264000  | -5.047781000 | -0.248806000 |
| C | 0.220602000  | -4.274540000 | -0.105220000 |
| H | 0.322644000  | -3.213039000 | 0.104156000  |
| C | -1.117955000 | -4.784146000 | -0.126765000 |
| C | -1.321573000 | -6.255135000 | -0.409193000 |
| H | -1.474622000 | -6.783458000 | 0.540528000  |
| C | -0.123900000 | -6.849566000 | -1.151283000 |
| C | 1.195139000  | -6.540504000 | -0.443966000 |
| H | 2.035297000  | -6.933852000 | -1.022602000 |
| C | -2.099451000 | -3.863845000 | 0.133663000  |
| H | -1.754609000 | -2.847528000 | 0.297185000  |
| C | -3.523400000 | -4.041187000 | 0.278016000  |
| C | -4.053983000 | -5.370320000 | 0.432721000  |
| N | -4.496950000 | -6.430555000 | 0.575994000  |
| C | -4.410856000 | -2.985390000 | 0.355852000  |
| C | -3.995175000 | -1.619700000 | 0.135363000  |
| H | -2.999166000 | -1.433832000 | -0.251677000 |
| C | -4.810194000 | -0.543238000 | 0.316680000  |
| C | -6.206490000 | -0.699152000 | 0.859975000  |
| H | -6.413858000 | 0.095937000  | 1.581054000  |
| C | -6.414361000 | -2.066010000 | 1.509887000  |
| C | -5.876219000 | -3.193203000 | 0.626795000  |
| H | -6.403875000 | -3.188272000 | -0.337854000 |
| C | -4.242316000 | 0.752118000  | -0.028244000 |
| H | -3.197417000 | 0.723380000  | -0.328413000 |
| C | -4.814597000 | 1.981796000  | -0.057732000 |
| C | -6.223995000 | 2.179192000  | 0.164780000  |
| N | -7.352404000 | 2.388159000  | 0.318562000  |
| C | -4.034162000 | 3.199824000  | -0.379379000 |
| C | -2.747701000 | 3.297999000  | 0.023162000  |
| H | -2.328778000 | 2.524416000  | 0.663320000  |
| C | -1.867895000 | 4.403754000  | -0.338973000 |
| C | -2.451309000 | 5.422399000  | -1.285454000 |
| H | -1.926899000 | 6.374626000  | -1.238768000 |
| C | -3.944861000 | 5.622769000  | -1.020483000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -4.707925000 | 4.307799000  | -1.149966000 |
| H | -5.738372000 | 4.424514000  | -0.799010000 |
| C | 0.154851000  | 6.721466000  | -0.216572000 |
| N | -0.066943000 | 7.847577000  | -0.370558000 |
| H | 7.300501000  | -0.116595000 | -0.211286000 |
| H | 4.790189000  | 6.466646000  | 1.121142000  |
| H | 3.618339000  | 5.609039000  | 2.116460000  |
| H | -4.348349000 | 6.359568000  | -1.718366000 |
| H | -4.080598000 | 6.023772000  | -0.010418000 |
| H | -5.899332000 | -2.092211000 | 2.476377000  |
| H | -7.476758000 | -2.225064000 | 1.706085000  |
| H | -0.250339000 | -7.930474000 | -1.243170000 |
| H | -0.085673000 | -6.440528000 | -2.167105000 |
| H | 7.590942000  | -2.617838000 | -0.329039000 |
| H | 6.542539000  | -1.993769000 | -1.598142000 |
| H | 2.472504000  | 7.071569000  | 0.443520000  |
| H | 5.264246000  | 4.496061000  | -0.209442000 |
| H | 6.780291000  | -0.908192000 | 1.257944000  |
| H | 5.517228000  | -3.995504000 | -0.659683000 |
| H | 1.230387000  | -7.041320000 | 0.532950000  |
| H | -6.922154000 | -0.549059000 | 0.040078000  |
| H | -6.053197000 | -4.169740000 | 1.081354000  |
| H | -2.231916000 | -6.407632000 | -0.991626000 |
| H | -2.314362000 | 5.033649000  | -2.304906000 |
| H | -4.779588000 | 4.006412000  | -2.204814000 |

#### VII[Cl<sup>-</sup>] (B3LYP)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.615672148 | 4.341027828  | 0.036371800  |
| H | -0.373550126 | 3.410453331  | 0.535232278  |
| C | 0.457424488  | 5.307377325  | 0.038667464  |
| C | 1.779118536  | 4.981548517  | 0.286327836  |
| C | 2.211149545  | 3.620527226  | 0.327998445  |
| H | 1.507252135  | 2.835988721  | 0.077832316  |
| C | 3.511862581  | 3.242826568  | 0.572482329  |
| C | 4.541587027  | 4.260755932  | 0.995209068  |
| H | 5.160905415  | 3.852468749  | 1.794017189  |
| C | 3.899353658  | 5.567694773  | 1.452255610  |
| C | 2.841014487  | 6.038857763  | 0.457115827  |
| H | 3.311955512  | 6.229864721  | -0.515541686 |
| C | 3.800883350  | 1.864686995  | 0.359463635  |
| H | 2.925993750  | 1.258998723  | 0.140888994  |
| C | 5.020314815  | 1.213832805  | 0.336016812  |
| C | 6.250908518  | 1.908296827  | 0.568923107  |
| N | 7.272793253  | 2.413241182  | 0.746663305  |
| C | 5.155375907  | -0.195883678 | 0.032394359  |
| C | 4.057949690  | -1.021869352 | -0.100708119 |
| H | 3.050457087  | -0.633859993 | 0.011206867  |
| C | 4.154718643  | -2.414418186 | -0.291423806 |
| C | 5.504414612  | -3.046515866 | -0.485681187 |
| H | 5.823470695  | -3.487232709 | 0.467208022  |
| C | 6.536183927  | -2.032059073 | -0.968263916 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 6.537141815  | -0.777969385 | -0.102797227 |
| C | 2.934503010  | -3.101249951 | -0.253737499 |
| H | 2.068285613  | -2.448919315 | -0.180633695 |
| C | 2.682440732  | -4.471124507 | -0.276042326 |
| C | 3.759981306  | -5.418774163 | -0.261334995 |
| N | 4.590764434  | -6.217742997 | -0.227108107 |
| C | 1.372311417  | -5.046584631 | -0.247781094 |
| C | 0.254312524  | -4.250926749 | -0.086015202 |
| H | 0.356608794  | -3.173165810 | 0.001119396  |
| C | -1.065802524 | -4.758031705 | 0.031075257  |
| C | -1.298572451 | -6.240714270 | -0.127219771 |
| H | -1.371430725 | -6.702398401 | 0.863680694  |
| C | -0.172992681 | -6.897638653 | -0.924095019 |
| C | 1.198617540  | -6.544703720 | -0.355612058 |
| H | 1.983596976  | -6.977045235 | -0.977159893 |
| C | -2.030444594 | -3.811555654 | 0.294303086  |
| H | -1.656640967 | -2.794031247 | 0.327773149  |
| C | -3.430380923 | -3.971284076 | 0.541198689  |
| C | -3.978517710 | -5.272583858 | 0.774433139  |
| N | -4.452618074 | -6.303480977 | 0.983935555  |
| C | -4.324541093 | -2.902211126 | 0.593013907  |
| C | -3.912772724 | -1.564707115 | 0.324372431  |
| H | -2.866828188 | -1.384424533 | 0.112400914  |
| C | -4.773217661 | -0.497975283 | 0.279277620  |
| C | -6.222485785 | -0.666249506 | 0.647838453  |
| H | -6.574690115 | 0.212654680  | 1.186713013  |
| C | -6.446322620 | -1.917557370 | 1.491706939  |
| C | -5.787161853 | -3.139904780 | 0.861857253  |
| H | -6.272924942 | -3.371939520 | -0.095661414 |
| C | -4.203222349 | 0.758101144  | -0.117501427 |
| H | -3.128257992 | 0.725737422  | -0.255358073 |
| C | -4.797025823 | 1.965704837  | -0.355133216 |
| C | -6.219963071 | 2.111294792  | -0.396701523 |
| N | -7.360123834 | 2.275057582  | -0.462601200 |
| C | -4.023344861 | 3.187380926  | -0.628085188 |
| C | -2.737466111 | 3.283994471  | -0.212137721 |
| H | -2.302015434 | 2.475688032  | 0.363714620  |
| C | -1.877584057 | 4.412991291  | -0.471616711 |
| C | -2.448921653 | 5.509544146  | -1.331761979 |
| H | -1.952066260 | 6.460104077  | -1.166385794 |
| C | -3.956617028 | 5.652326129  | -1.117002637 |
| C | -4.683070204 | 4.331621067  | -1.356961483 |
| H | -5.729034230 | 4.417663559  | -1.057399011 |
| C | 0.168413459  | 6.699067567  | -0.127624537 |
| N | -0.029552242 | 7.830369557  | -0.239985687 |
| H | 7.224992620  | -0.035296086 | -0.508240514 |
| H | 4.666645033  | 6.333282336  | 1.577522043  |
| H | 3.429366067  | 5.422339966  | 2.429876231  |
| H | -4.355395656 | 6.424078808  | -1.777621767 |
| H | -4.141000215 | 5.983514874  | -0.090536031 |
| H | -6.023748868 | -1.758665970 | 2.488523444  |
| H | -7.514999035 | -2.094862197 | 1.621826640  |



|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -0.307729319 | -7.980469959 | -0.932402414 |
| H  | -0.223785992 | -6.560475326 | -1.964329899 |
| H  | 7.528946940  | -2.484572692 | -0.975588230 |
| H  | 6.304531641  | -1.749326387 | -1.999820777 |
| H  | 2.401807626  | 6.982572724  | 0.777321099  |
| H  | 5.225186579  | 4.451546538  | 0.161305536  |
| H  | 6.913420763  | -1.007777066 | 0.903565172  |
| H  | 5.443314416  | -3.876660692 | -1.186602665 |
| H  | 1.320046942  | -6.994558617 | 0.637796508  |
| H  | -6.823956873 | -0.708633582 | -0.267443585 |
| H  | -5.924473719 | -4.020983192 | 1.488171190  |
| H  | -2.253291163 | -6.429228044 | -0.614329870 |
| H  | -2.257539632 | 5.237186453  | -2.377925947 |
| H  | -4.700757252 | 4.098408808  | -2.429751630 |
| Cl | 0.448400898  | -0.380746571 | 0.073137288  |

### VII[Cl] (M06-2X)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.630998000 | 4.463810000  | 0.343415000  |
| H | -0.407302000 | 3.596619000  | 0.953979000  |
| C | 0.446776000  | 5.446265000  | 0.269196000  |
| C | 1.763110000  | 5.112413000  | 0.362227000  |
| C | 2.173251000  | 3.726898000  | 0.361647000  |
| H | 1.434106000  | 2.958960000  | 0.164038000  |
| C | 3.462488000  | 3.330590000  | 0.522819000  |
| C | 4.543752000  | 4.316390000  | 0.874779000  |
| H | 5.178697000  | 3.899116000  | 1.656458000  |
| C | 3.973163000  | 5.651949000  | 1.334469000  |
| C | 2.866947000  | 6.130983000  | 0.401074000  |
| H | 3.271462000  | 6.247952000  | -0.610821000 |
| C | 3.715366000  | 1.926164000  | 0.306226000  |
| H | 2.822277000  | 1.341279000  | 0.108669000  |
| C | 4.896790000  | 1.255818000  | 0.260446000  |
| C | 6.152683000  | 1.930451000  | 0.460264000  |
| N | 7.187544000  | 2.406072000  | 0.604254000  |
| C | 5.011137000  | -0.178482000 | -0.028957000 |
| C | 3.930018000  | -1.001060000 | -0.066425000 |
| H | 2.922180000  | -0.627680000 | 0.089987000  |
| C | 4.034019000  | -2.420697000 | -0.232091000 |
| C | 5.391264000  | -3.024008000 | -0.452515000 |
| H | 5.777912000  | -3.366811000 | 0.514979000  |
| C | 6.350824000  | -2.015918000 | -1.067720000 |
| C | 6.391936000  | -0.728400000 | -0.265474000 |
| C | 2.845395000  | -3.113338000 | -0.146024000 |
| H | 1.962889000  | -2.490425000 | -0.038074000 |
| C | 2.632226000  | -4.508404000 | -0.158200000 |
| C | 3.748061000  | -5.419526000 | -0.085155000 |
| N | 4.597693000  | -6.185667000 | 0.003895000  |
| C | 1.371157000  | -5.123766000 | -0.165180000 |
| C | 0.219828000  | -4.334287000 | -0.147508000 |
| H | 0.291759000  | -3.250021000 | -0.161388000 |
| C | -1.079412000 | -4.859032000 | -0.065258000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -1.294344000 | -6.348586000 | -0.124081000 |
| H | -1.440497000 | -6.739366000 | 0.888029000  |
| C | -0.104819000 | -7.037679000 | -0.785180000 |
| C | 1.216364000  | -6.624269000 | -0.148732000 |
| H | 2.049216000  | -7.097864000 | -0.668227000 |
| C | -2.046581000 | -3.882610000 | 0.100821000  |
| H | -1.659134000 | -2.867353000 | 0.080258000  |
| C | -3.437140000 | -4.020063000 | 0.341275000  |
| C | -4.021435000 | -5.320441000 | 0.527282000  |
| N | -4.522003000 | -6.340283000 | 0.692680000  |
| C | -4.287595000 | -2.925174000 | 0.440318000  |
| C | -3.827657000 | -1.588029000 | 0.236215000  |
| H | -2.786431000 | -1.396165000 | -0.001505000 |
| C | -4.666156000 | -0.512918000 | 0.264075000  |
| C | -6.108025000 | -0.650144000 | 0.656644000  |
| H | -6.410434000 | 0.209507000  | 1.253489000  |
| C | -6.354596000 | -1.935778000 | 1.428956000  |
| C | -5.751415000 | -3.128060000 | 0.703339000  |
| H | -6.243322000 | -3.254863000 | -0.270227000 |
| C | -4.072409000 | 0.758694000  | -0.084831000 |
| H | -2.993456000 | 0.734158000  | -0.208539000 |
| C | -4.678469000 | 1.950322000  | -0.300010000 |
| C | -6.110006000 | 2.084100000  | -0.344892000 |
| N | -7.244765000 | 2.243119000  | -0.414115000 |
| C | -3.920362000 | 3.188526000  | -0.552764000 |
| C | -2.707356000 | 3.343031000  | 0.005024000  |
| H | -2.325558000 | 2.585379000  | 0.680665000  |
| C | -1.839422000 | 4.479334000  | -0.251096000 |
| C | -2.342466000 | 5.501204000  | -1.234543000 |
| H | -1.887032000 | 6.474090000  | -1.071811000 |
| C | -3.863096000 | 5.610806000  | -1.177958000 |
| C | -4.525430000 | 4.261271000  | -1.419878000 |
| H | -5.598879000 | 4.328213000  | -1.234450000 |
| C | 0.118778000  | 6.841465000  | 0.178462000  |
| N | -0.130895000 | 7.961089000  | 0.121233000  |
| H | 7.003363000  | 0.016491000  | -0.775463000 |
| H | 4.770748000  | 6.392714000  | 1.386265000  |
| H | 3.565171000  | 5.544721000  | 2.342784000  |
| H | -4.212161000 | 6.334414000  | -1.914506000 |
| H | -4.158507000 | 5.982449000  | -0.193614000 |
| H | -5.901528000 | -1.853903000 | 2.420029000  |
| H | -7.423869000 | -2.088233000 | 1.571549000  |
| H | -0.224222000 | -8.119122000 | -0.725111000 |
| H | -0.083519000 | -6.772643000 | -1.845706000 |
| H | 7.348529000  | -2.448733000 | -1.136746000 |
| H | 6.024421000  | -1.788052000 | -2.085637000 |
| H | 2.486424000  | 7.103181000  | 0.709288000  |
| H | 5.197639000  | 4.459796000  | 0.008362000  |
| H | 6.873699000  | -0.892749000 | 0.706586000  |
| H | 5.328388000  | -3.904320000 | -1.085951000 |
| H | 1.259142000  | -6.977754000 | 0.887779000  |
| H | -6.729357000 | -0.619068000 | -0.245971000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -5.917132000 | -4.052291000 | 1.254188000  |
| H  | -2.204919000 | -6.579525000 | -0.672956000 |
| H  | -2.041785000 | 5.173235000  | -2.236408000 |
| H  | -4.415857000 | 3.967321000  | -2.470412000 |
| Cl | 0.009371000  | -0.805107000 | 0.069760000  |

VII[SO<sub>4</sub><sup>2-</sup>] (B3LYP)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.575974234 | 4.203644516  | -0.102077502 |
| H | -0.316743211 | 3.257412202  | 0.368500746  |
| C | 0.443904873  | 5.174375197  | -0.096143273 |
| C | 1.788686526  | 4.877667923  | 0.244105161  |
| C | 2.233223572  | 3.559089312  | 0.240241608  |
| H | 1.550949840  | 2.767981200  | -0.043515878 |
| C | 3.575446993  | 3.192853651  | 0.494293974  |
| C | 4.560778009  | 4.247380960  | 0.946667713  |
| H | 5.236151587  | 3.838429026  | 1.696046756  |
| C | 3.853249095  | 5.478616763  | 1.507808832  |
| C | 2.773439494  | 5.982511413  | 0.553806271  |
| H | 3.235343989  | 6.333883957  | -0.377516044 |
| C | 3.877751404  | 1.861751011  | 0.278615376  |
| H | 3.029280427  | 1.249180831  | -0.004226919 |
| C | 5.134004607  | 1.189230255  | 0.327482730  |
| C | 6.349830333  | 1.909599679  | 0.558154517  |
| N | 7.356777786  | 2.447390383  | 0.732429978  |
| C | 5.269118570  | -0.187083751 | 0.107523648  |
| C | 4.140395247  | -1.028575273 | -0.070988294 |
| H | 3.134075261  | -0.630502277 | 0.038028382  |
| C | 4.233132895  | -2.384639528 | -0.276827258 |
| C | 5.567431325  | -3.059507568 | -0.450584459 |
| H | 5.834096933  | -3.576941739 | 0.478796923  |
| C | 6.656188725  | -2.057354698 | -0.821448329 |
| C | 6.628284629  | -0.838169547 | 0.099905913  |
| C | 2.979719435  | -3.074166740 | -0.307608432 |
| H | 2.124053199  | -2.405116729 | -0.321089335 |
| C | 2.704366929  | -4.412869318 | -0.281192906 |
| C | 3.738033694  | -5.402090148 | -0.214948518 |
| N | 4.529481298  | -6.240278261 | -0.147156155 |
| C | 1.336584451  | -4.947597933 | -0.278426206 |
| C | 0.275012103  | -4.171126847 | 0.052979359  |
| H | 0.425975587  | -3.131489330 | 0.327524089  |
| C | -1.083341307 | -4.650679618 | 0.123367228  |
| C | -1.325583550 | -6.108852413 | -0.184945106 |
| H | -1.294527703 | -6.685102650 | 0.746590865  |
| C | -0.275852005 | -6.650631816 | -1.154186912 |
| C | 1.139359193  | -6.401114390 | -0.642485682 |
| H | 1.869645515  | -6.700345806 | -1.397702890 |
| C | -2.036126262 | -3.745331376 | 0.474265229  |
| H | -1.691685355 | -2.723189309 | 0.590124564  |
| C | -3.451365423 | -3.950978626 | 0.695067574  |
| C | -3.943777034 | -5.262028421 | 0.991919831  |
| N | -4.366296457 | -6.304357816 | 1.254282428  |
| C | -4.380209946 | -2.926436546 | 0.699983822  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -3.987821440 | -1.589613789 | 0.388818435  |
| H | -2.955778622 | -1.368272750 | 0.141797801  |
| C | -4.854183182 | -0.528383215 | 0.344685469  |
| C | -6.302867077 | -0.696506296 | 0.725683864  |
| H | -6.659925423 | 0.186734837  | 1.255995090  |
| C | -6.503701546 | -1.940901621 | 1.591089159  |
| C | -5.844854262 | -3.172249717 | 0.970266960  |
| H | -6.340963912 | -3.406958719 | 0.018838003  |
| C | -4.256611848 | 0.706654860  | -0.053467179 |
| H | -3.172646025 | 0.646994138  | -0.146566606 |
| C | -4.836381417 | 1.921284908  | -0.337857170 |
| C | -6.256054553 | 2.067874011  | -0.431486375 |
| N | -7.395826740 | 2.219441028  | -0.542632664 |
| C | -4.039772496 | 3.106690781  | -0.624802410 |
| C | -2.718044336 | 3.174292510  | -0.269744603 |
| H | -2.258309339 | 2.364032926  | 0.284681062  |
| C | -1.873636584 | 4.273075847  | -0.585120289 |
| C | -2.437481002 | 5.348410683  | -1.470884684 |
| H | -1.896199842 | 6.284630657  | -1.392815886 |
| C | -3.922906829 | 5.564988695  | -1.183263069 |
| C | -4.703070515 | 4.264288685  | -1.327388007 |
| H | -5.725365888 | 4.387315599  | -0.963548285 |
| C | 0.178587189  | 6.557143983  | -0.365255128 |
| N | 0.031634850  | 7.686069143  | -0.558287142 |
| H | 7.403644578  | -0.127162350 | -0.183404627 |
| H | 4.581759255  | 6.268358248  | 1.705171282  |
| H | 3.387632029  | 5.223654001  | 2.465293847  |
| H | -4.331357829 | 6.324549148  | -1.853662289 |
| H | -4.032418789 | 5.946124469  | -0.162733822 |
| H | -6.064465704 | -1.763747147 | 2.578189509  |
| H | -7.570559675 | -2.121196605 | 1.741678588  |
| H | -0.436866214 | -7.718843198 | -1.318913056 |
| H | -0.393183558 | -6.153420769 | -2.122418943 |
| H | 7.638183320  | -2.533152902 | -0.775057048 |
| H | 6.507708584  | -1.724865632 | -1.853900060 |
| H | 2.259777884  | 6.843548652  | 0.982425612  |
| H | 5.192457339  | 4.540716345  | 0.100634797  |
| H | 6.860333369  | -1.151808641 | 1.126870656  |
| H | 5.498137306  | -3.842389007 | -1.206236445 |
| H | 1.340959984  | -7.032462689 | 0.232034553  |
| H | -6.915445997 | -0.763109010 | -0.180471145 |
| H | -5.980626194 | -4.045241295 | 1.608841699  |
| H | -2.320648047 | -6.257201557 | -0.600209950 |
| H | -2.315638771 | 5.003471654  | -2.507012988 |
| H | -4.802310704 | 4.001169781  | -2.389775397 |
| O | 0.363459896  | 1.231861678  | -1.144331177 |
| S | 0.062863422  | 0.412486093  | 0.063970741  |
| O | -1.245970352 | -0.285547252 | -0.077705423 |
| O | 1.147343121  | -0.587302350 | 0.289625169  |
| O | -0.006212318 | 1.356508872  | 1.225205230  |

VII[SO<sub>4</sub><sup>-2</sup>] (M06-2X)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.571648000 | 4.210048000  | -0.017930000 |
| H | -0.302937000 | 3.227624000  | 0.373230000  |
| C | 0.446078000  | 5.167851000  | -0.011625000 |
| C | 1.791495000  | 4.868626000  | 0.305895000  |
| C | 2.211656000  | 3.549036000  | 0.252995000  |
| H | 1.519884000  | 2.762597000  | -0.049187000 |
| C | 3.564924000  | 3.170656000  | 0.440970000  |
| C | 4.572581000  | 4.203444000  | 0.884001000  |
| H | 5.273661000  | 3.767695000  | 1.594143000  |
| C | 3.888043000  | 5.410229000  | 1.515115000  |
| C | 2.788190000  | 5.958245000  | 0.614723000  |
| H | 3.222409000  | 6.342077000  | -0.315698000 |
| C | 3.826260000  | 1.855373000  | 0.156990000  |
| H | 2.957005000  | 1.254862000  | -0.100896000 |
| C | 5.099363000  | 1.192574000  | 0.118898000  |
| C | 6.318467000  | 1.949269000  | 0.211687000  |
| N | 7.320294000  | 2.511164000  | 0.260115000  |
| C | 5.234947000  | -0.168964000 | -0.064453000 |
| C | 4.090754000  | -1.028080000 | -0.136730000 |
| H | 3.086307000  | -0.633078000 | 0.003103000  |
| C | 4.197834000  | -2.375361000 | -0.284637000 |
| C | 5.519345000  | -3.055045000 | -0.502604000 |
| H | 5.845634000  | -3.523006000 | 0.433166000  |
| C | 6.566115000  | -2.066316000 | -0.996420000 |
| C | 6.591645000  | -0.814125000 | -0.130616000 |
| C | 2.939797000  | -3.086067000 | -0.231375000 |
| H | 2.073199000  | -2.428251000 | -0.267189000 |
| C | 2.703513000  | -4.411557000 | -0.113409000 |
| C | 3.764960000  | -5.376551000 | 0.001080000  |
| N | 4.568024000  | -6.191785000 | 0.111807000  |
| C | 1.340379000  | -4.972896000 | -0.062307000 |
| C | 0.289478000  | -4.194797000 | 0.249714000  |
| H | 0.425850000  | -3.142211000 | 0.487297000  |
| C | -1.079700000 | -4.679567000 | 0.302047000  |
| C | -1.307274000 | -6.145180000 | 0.035220000  |
| H | -1.273399000 | -6.691483000 | 0.984545000  |
| C | -0.245697000 | -6.701623000 | -0.909336000 |
| C | 1.160795000  | -6.433199000 | -0.392688000 |
| H | 1.900119000  | -6.738487000 | -1.136490000 |
| C | -2.028176000 | -3.759112000 | 0.569212000  |
| H | -1.683127000 | -2.736660000 | 0.689267000  |
| C | -3.465062000 | -3.960581000 | 0.693852000  |
| C | -3.963367000 | -5.258214000 | 1.064670000  |
| N | -4.383311000 | -6.278629000 | 1.387506000  |
| C | -4.383414000 | -2.961239000 | 0.551087000  |
| C | -3.952607000 | -1.629849000 | 0.196634000  |
| H | -2.907446000 | -1.444652000 | -0.031601000 |
| C | -4.802392000 | -0.572392000 | 0.121117000  |
| C | -6.259982000 | -0.701670000 | 0.479723000  |
| H | -6.590576000 | 0.191344000  | 1.010902000  |
| C | -6.507094000 | -1.936156000 | 1.338790000  |
| C | -5.862428000 | -3.174166000 | 0.724754000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -6.304480000 | -3.357739000 | -0.261925000 |
| C | -4.172486000 | 0.670342000  | -0.235977000 |
| H | -3.080678000 | 0.612745000  | -0.271545000 |
| C | -4.760493000 | 1.870430000  | -0.517057000 |
| C | -6.179896000 | 1.977245000  | -0.717368000 |
| N | -7.305235000 | 2.103224000  | -0.917445000 |
| C | -3.990215000 | 3.096203000  | -0.680382000 |
| C | -2.689780000 | 3.169831000  | -0.264441000 |
| H | -2.201628000 | 2.322886000  | 0.211095000  |
| C | -1.891468000 | 4.334159000  | -0.432377000 |
| C | -2.503796000 | 5.547411000  | -1.070247000 |
| H | -2.059487000 | 6.462491000  | -0.692999000 |
| C | -4.011953000 | 5.588584000  | -0.871167000 |
| C | -4.660471000 | 4.287222000  | -1.306380000 |
| H | -5.724462000 | 4.289617000  | -1.069487000 |
| C | 0.208471000  | 6.563350000  | -0.295462000 |
| N | 0.100858000  | 7.687707000  | -0.505198000 |
| H | 7.337335000  | -0.105742000 | -0.489413000 |
| H | 4.626400000  | 6.185572000  | 1.723922000  |
| H | 3.444567000  | 5.113868000  | 2.469632000  |
| H | -4.437629000 | 6.427653000  | -1.422876000 |
| H | -4.226352000 | 5.754178000  | 0.188080000  |
| H | -6.081016000 | -1.772966000 | 2.332524000  |
| H | -7.578895000 | -2.094717000 | 1.466079000  |
| H | -0.399535000 | -7.773037000 | -1.048511000 |
| H | -0.356950000 | -6.226333000 | -1.887862000 |
| H | 7.552085000  | -2.532576000 | -1.005841000 |
| H | 6.330909000  | -1.780922000 | -2.025411000 |
| H | 2.290977000  | 6.802518000  | 1.093637000  |
| H | 5.170814000  | 4.525880000  | 0.025913000  |
| H | 6.882350000  | -1.082182000 | 0.893276000  |
| H | 5.404189000  | -3.870213000 | -1.217056000 |
| H | 1.363296000  | -7.039954000 | 0.497826000  |
| H | -6.864771000 | -0.747245000 | -0.431953000 |
| H | -6.058977000 | -4.058695000 | 1.329929000  |
| H | -2.296517000 | -6.315657000 | -0.384164000 |
| H | -2.270858000 | 5.507428000  | -2.142150000 |
| H | -4.594344000 | 4.174824000  | -2.396638000 |
| O | 0.529993000  | 1.267047000  | -1.049463000 |
| S | 0.078674000  | 0.469971000  | 0.117812000  |
| O | -1.221209000 | -0.192739000 | -0.170111000 |
| O | 1.101006000  | -0.563742000 | 0.427008000  |
| O | -0.089051000 | 1.396780000  | 1.263401000  |

#### VIII (M06-2X)

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -0.624074000 | 3.974150000 | -0.610217000 |
| H | -0.379241000 | 2.917583000 | -0.708472000 |
| C | 0.385206000  | 4.934571000 | -1.010560000 |
| C | 1.751704000  | 4.674572000 | -1.000884000 |
| N | 2.236941000  | 3.505368000 | -0.485303000 |
| H | 1.552312000  | 2.865670000 | -0.101237000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 3.566652000  | 3.111170000  | -0.335134000 |
| C | 4.604243000  | 4.114746000  | -0.779095000 |
| H | 5.502168000  | 4.019340000  | -0.171687000 |
| C | 4.080084000  | 5.552117000  | -0.740272000 |
| C | 2.771374000  | 5.652152000  | -1.525498000 |
| H | 2.960760000  | 5.426811000  | -2.585076000 |
| C | 3.789684000  | 1.851127000  | 0.148353000  |
| H | 2.929933000  | 1.197232000  | 0.270730000  |
| C | 5.028225000  | 1.209757000  | 0.506258000  |
| C | 6.230598000  | 1.967827000  | 0.688925000  |
| N | 7.221642000  | 2.557241000  | 0.858591000  |
| C | 5.134132000  | -0.165693000 | 0.736048000  |
| N | 4.022724000  | -0.928628000 | 0.519074000  |
| C | 4.075618000  | -2.247636000 | 0.587287000  |
| C | 5.310252000  | -3.000521000 | 1.045625000  |
| H | 5.015478000  | -3.892250000 | 1.603006000  |
| C | 6.205427000  | -2.100105000 | 1.897512000  |
| C | 6.452364000  | -0.786454000 | 1.158288000  |
| C | 2.859826000  | -2.917716000 | 0.208127000  |
| H | 1.986560000  | -2.280314000 | 0.110471000  |
| C | 2.665336000  | -4.246165000 | -0.100419000 |
| C | 3.752296000  | -5.182062000 | -0.154151000 |
| N | 4.601579000  | -5.975796000 | -0.228737000 |
| C | 1.343895000  | -4.803647000 | -0.434703000 |
| N | 0.298031000  | -4.045519000 | -0.251480000 |
| C | -0.984506000 | -4.544722000 | -0.401812000 |
| C | -1.201566000 | -5.976073000 | -0.855110000 |
| H | -1.312131000 | -6.628812000 | 0.021718000  |
| C | -0.025592000 | -6.460574000 | -1.705028000 |
| C | 1.279257000  | -6.230198000 | -0.948291000 |
| H | 2.147620000  | -6.440304000 | -1.579271000 |
| C | -1.990749000 | -3.658452000 | -0.090143000 |
| H | -1.688444000 | -2.640059000 | 0.126465000  |
| C | -3.400936000 | -3.909070000 | 0.029760000  |
| C | -3.896606000 | -5.254369000 | 0.105782000  |
| N | -4.323862000 | -6.334428000 | 0.198013000  |
| C | -4.353940000 | -2.894722000 | 0.187602000  |
| N | -3.921175000 | -1.602342000 | 0.139130000  |
| C | -4.769062000 | -0.592682000 | 0.234232000  |
| C | -6.275683000 | -0.767532000 | 0.270952000  |
| H | -6.627016000 | -0.617069000 | 1.300792000  |
| C | -6.691756000 | -2.150558000 | -0.228940000 |
| C | -5.813658000 | -3.214979000 | 0.429787000  |
| H | -6.057896000 | -4.215223000 | 0.067673000  |
| C | -4.144581000 | 0.702965000  | 0.266655000  |
| H | -3.077416000 | 0.701073000  | 0.069654000  |
| C | -4.693553000 | 1.937496000  | 0.531503000  |
| C | -6.067004000 | 2.103639000  | 0.911017000  |
| N | -7.169287000 | 2.290555000  | 1.238226000  |
| C | -3.903172000 | 3.180891000  | 0.460037000  |
| N | -2.674879000 | 3.090344000  | 0.037918000  |
| C | -1.895206000 | 4.218012000  | -0.160888000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -2.456634000 | 5.599153000  | 0.108685000  |
| H | -1.657176000 | 6.288946000  | 0.384624000  |
| C | -3.519181000 | 5.539391000  | 1.209466000  |
| C | -4.568333000 | 4.485067000  | 0.860610000  |
| H | -5.250695000 | 4.315587000  | 1.698418000  |
| C | -0.016105000 | 6.203589000  | -1.533589000 |
| N | -0.340546000 | 7.230157000  | -1.981739000 |
| H | 7.061719000  | -0.977837000 | 0.262499000  |
| H | 4.825984000  | 6.229065000  | -1.165412000 |
| H | 3.916608000  | 5.865900000  | 0.297316000  |
| H | -3.988554000 | 6.518572000  | 1.340966000  |
| H | -3.045825000 | 5.279477000  | 2.164204000  |
| H | -7.748431000 | -2.330461000 | -0.011646000 |
| H | -6.574115000 | -2.203218000 | -1.318010000 |
| H | -0.145810000 | -7.518800000 | -1.954070000 |
| H | -0.001070000 | -5.907658000 | -2.651986000 |
| H | 5.717030000  | -1.896409000 | 2.858109000  |
| H | 7.151260000  | -2.602876000 | 2.118026000  |
| H | 2.355690000  | 6.660804000  | -1.495597000 |
| H | 4.902238000  | 3.865364000  | -1.807645000 |
| H | 7.025525000  | -0.087434000 | 1.771937000  |
| H | 5.866352000  | -3.365096000 | 0.171742000  |
| H | 1.354585000  | -6.922595000 | -0.096806000 |
| H | -6.754581000 | 0.016729000  | -0.319903000 |
| H | -5.999018000 | -3.223962000 | 1.514414000  |
| H | -2.133259000 | -6.062786000 | -1.414922000 |
| H | -2.900834000 | 6.002390000  | -0.811629000 |
| H | -5.198770000 | 4.833175000  | 0.029135000  |

### VIII[Cl](M06-2X)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.733656000 | 4.045357000  | -0.008250000 |
| H | -0.489109000 | 2.989557000  | -0.139229000 |
| C | 0.322623000  | 4.989100000  | -0.194113000 |
| C | 1.691610000  | 4.668953000  | -0.355658000 |
| N | 2.176591000  | 3.408985000  | -0.262193000 |
| H | 1.512785000  | 2.585612000  | -0.095898000 |
| C | 3.516193000  | 3.038785000  | -0.330400000 |
| C | 4.527704000  | 4.111050000  | -0.667624000 |
| H | 4.995124000  | 4.485418000  | 0.253196000  |
| C | 3.884425000  | 5.273428000  | -1.416926000 |
| C | 2.687557000  | 5.780016000  | -0.619424000 |
| H | 2.189409000  | 6.603002000  | -1.133290000 |
| C | 3.815150000  | 1.714300000  | -0.100990000 |
| H | 2.977400000  | 1.030635000  | 0.036228000  |
| C | 5.106303000  | 1.107473000  | 0.002152000  |
| C | 6.306144000  | 1.890270000  | 0.089721000  |
| N | 7.298019000  | 2.496470000  | 0.186726000  |
| C | 5.279769000  | -0.287441000 | 0.121364000  |
| N | 4.172240000  | -1.058080000 | 0.080478000  |
| C | 4.226503000  | -2.380661000 | 0.176504000  |
| C | 5.543189000  | -3.141098000 | 0.200403000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| H | 5.764263000  | -3.457631000 | 1.228807000  |
| C | 6.689884000  | -2.283316000 | -0.338383000 |
| C | 6.653086000  | -0.900706000 | 0.315275000  |
| C | 2.950896000  | -3.022844000 | 0.224102000  |
| H | 2.099929000  | -2.363814000 | 0.066928000  |
| C | 2.652383000  | -4.355716000 | 0.467633000  |
| C | 3.663810000  | -5.311603000 | 0.816734000  |
| N | 4.440882000  | -6.126239000 | 1.121363000  |
| C | 1.291412000  | -4.891873000 | 0.401977000  |
| N | 0.323333000  | -4.083765000 | 0.055271000  |
| C | -0.954780000 | -4.538793000 | -0.174918000 |
| C | -1.263600000 | -6.020154000 | -0.052742000 |
| H | -2.316020000 | -6.178766000 | 0.182556000  |
| C | -0.380266000 | -6.653356000 | 1.025178000  |
| C | 1.086638000  | -6.365769000 | 0.720440000  |
| H | 1.421191000  | -6.968060000 | -0.137435000 |
| C | -1.888239000 | -3.571665000 | -0.491031000 |
| H | -1.565795000 | -2.537386000 | -0.404698000 |
| C | -3.245571000 | -3.762329000 | -0.915331000 |
| C | -3.666196000 | -5.022573000 | -1.456225000 |
| N | -4.023985000 | -6.026148000 | -1.931700000 |
| C | -4.211191000 | -2.737717000 | -0.911237000 |
| N | -3.857228000 | -1.517250000 | -0.452486000 |
| C | -4.757972000 | -0.564601000 | -0.236627000 |
| C | -6.256805000 | -0.826414000 | -0.283135000 |
| H | -6.733968000 | -0.404768000 | 0.604880000  |
| C | -6.590064000 | -2.313667000 | -0.411040000 |
| C | -5.624381000 | -2.975893000 | -1.398488000 |
| H | -5.745037000 | -2.517953000 | -2.391476000 |
| C | -4.214533000 | 0.726205000  | 0.035861000  |
| H | -3.128748000 | 0.782360000  | 0.017987000  |
| C | -4.864379000 | 1.928582000  | 0.283240000  |
| C | -6.293044000 | 2.043000000  | 0.361102000  |
| N | -7.445813000 | 2.202720000  | 0.433238000  |
| C | -4.138239000 | 3.183853000  | 0.452677000  |
| N | -2.844281000 | 3.154929000  | 0.257608000  |
| C | -2.064568000 | 4.276997000  | 0.306056000  |
| C | -2.673032000 | 5.619499000  | 0.675338000  |
| H | -1.950599000 | 6.231916000  | 1.217600000  |
| C | -3.939893000 | 5.428715000  | 1.515769000  |
| C | -4.890444000 | 4.450827000  | 0.823046000  |
| H | -5.747924000 | 4.216460000  | 1.460660000  |
| C | 0.025814000  | 6.388651000  | -0.289715000 |
| N | -0.191619000 | 7.530607000  | -0.394049000 |
| H | 7.433066000  | -0.249683000 | -0.086303000 |
| H | 3.555469000  | 4.946616000  | -2.410753000 |
| H | 4.611400000  | 6.077983000  | -1.565497000 |
| H | -4.432779000 | 6.391705000  | 1.686040000  |
| H | -3.668048000 | 5.028662000  | 2.500603000  |
| H | -6.494963000 | -2.805262000 | 0.564942000  |
| H | -7.628907000 | -2.441998000 | -0.732493000 |
| H | -0.640031000 | -6.230444000 | 2.003626000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -0.558006000 | -7.732263000 | 1.084106000  |
| H  | 7.650748000  | -2.775438000 | -0.155585000 |
| H  | 6.587958000  | -2.171911000 | -1.425153000 |
| H  | 3.033136000  | 6.185026000  | 0.343216000  |
| H  | 5.334356000  | 3.676049000  | -1.257852000 |
| H  | 6.856964000  | -0.999522000 | 1.392323000  |
| H  | 5.454237000  | -4.063171000 | -0.378263000 |
| H  | 1.728280000  | -6.660455000 | 1.556222000  |
| H  | -6.680630000 | -0.273444000 | -1.132153000 |
| H  | -5.833915000 | -4.040497000 | -1.513158000 |
| H  | -1.085567000 | -6.522939000 | -1.013898000 |
| H  | -2.919076000 | 6.182589000  | -0.235672000 |
| H  | -5.307126000 | 4.910494000  | -0.085868000 |
| Cl | 0.515903000  | 0.868750000  | 0.097222000  |

### IX (M06-2X)

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.776757000 | 3.962103000  | 0.884975000  |
| H | -0.611188000 | 2.931537000  | 1.209548000  |
| C | 0.235577000  | 4.935905000  | 1.321401000  |
| C | 1.581532000  | 4.644677000  | 1.262531000  |
| N | 1.988654000  | 3.505434000  | 0.612632000  |
| H | 1.266946000  | 3.032481000  | 0.082596000  |
| C | 3.291826000  | 3.027984000  | 0.440522000  |
| C | 4.353370000  | 3.800643000  | 1.182683000  |
| H | 4.410396000  | 3.409827000  | 2.209285000  |
| C | 4.015201000  | 5.296584000  | 1.231265000  |
| C | 2.650133000  | 5.501561000  | 1.893527000  |
| H | 2.332831000  | 6.547210000  | 1.862251000  |
| C | 3.483912000  | 1.935618000  | -0.341859000 |
| H | 2.589594000  | 1.469490000  | -0.762815000 |
| C | 4.763087000  | 1.348642000  | -0.766070000 |
| C | 5.837161000  | 2.218329000  | -1.120572000 |
| N | 6.704251000  | 2.950116000  | -1.394875000 |
| C | 4.955892000  | -0.004669000 | -0.948567000 |
| N | 3.974387000  | -0.905336000 | -0.603007000 |
| C | 4.012624000  | -2.299602000 | -0.683291000 |
| C | 5.310127000  | -2.886328000 | -1.190672000 |
| H | 5.485667000  | -3.856888000 | -0.732626000 |
| C | 6.506712000  | -1.962355000 | -0.950953000 |
| C | 6.219763000  | -0.579155000 | -1.533812000 |
| C | 2.882904000  | -2.982416000 | -0.325888000 |
| H | 2.002853000  | -2.400728000 | -0.064098000 |
| C | 2.648993000  | -4.406132000 | -0.242528000 |
| C | 3.718211000  | -5.345521000 | -0.421487000 |
| N | 4.563834000  | -6.135674000 | -0.558740000 |
| C | 1.402301000  | -4.964193000 | 0.040833000  |
| N | 0.320911000  | -4.124922000 | 0.147367000  |
| C | -0.862970000 | -4.586955000 | 0.497894000  |
| C | -1.100579000 | -6.000157000 | 0.996988000  |
| H | -1.747457000 | -5.971311000 | 1.877848000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 0.207544000  | -6.725026000 | 1.309578000  |
| C | 1.212616000  | -6.458594000 | 0.187269000  |
| H | 0.820682000  | -6.866305000 | -0.756419000 |
| C | -1.943863000 | -3.635355000 | 0.365837000  |
| H | -1.639248000 | -2.639072000 | 0.061313000  |
| C | -3.297867000 | -3.813254000 | 0.514272000  |
| C | -3.881810000 | -5.078111000 | 0.855801000  |
| N | -4.412310000 | -6.080672000 | 1.121723000  |
| C | -4.270145000 | -2.714420000 | 0.282363000  |
| N | -3.799087000 | -1.561218000 | -0.077491000 |
| C | -4.642629000 | -0.492604000 | -0.375376000 |
| C | -6.144445000 | -0.673887000 | -0.349025000 |
| H | -6.641509000 | 0.278703000  | -0.156554000 |
| C | -6.534368000 | -1.715794000 | 0.703864000  |
| C | -5.747606000 | -3.007020000 | 0.476817000  |
| H | -6.123707000 | -3.533109000 | -0.412936000 |
| C | -4.006563000 | 0.674841000  | -0.676586000 |
| H | -2.920029000 | 0.612528000  | -0.632749000 |
| C | -4.566691000 | 1.956720000  | -1.086378000 |
| C | -5.779444000 | 2.011873000  | -1.835612000 |
| N | -6.762675000 | 2.058693000  | -2.461798000 |
| C | -3.915440000 | 3.153002000  | -0.829299000 |
| N | -2.802724000 | 3.162944000  | -0.034506000 |
| C | -1.909489000 | 4.217622000  | 0.188834000  |
| C | -2.312114000 | 5.558765000  | -0.368962000 |
| H | -2.874671000 | 6.109770000  | 0.397109000  |
| C | -3.172923000 | 5.411219000  | -1.630891000 |
| C | -4.368936000 | 4.489675000  | -1.356478000 |
| H | -5.021481000 | 4.957412000  | -0.605221000 |
| C | -0.184796000 | 6.166921000  | 1.901651000  |
| N | -0.563351000 | 7.172133000  | 2.358948000  |
| H | 6.100796000  | -0.660741000 | -2.623953000 |
| H | 4.009970000  | 5.706379000  | 0.214766000  |
| H | 4.784776000  | 5.836357000  | 1.789935000  |
| H | -2.571579000 | 4.999872000  | -2.450331000 |
| H | -3.527693000 | 6.393265000  | -1.955617000 |
| H | -6.312688000 | -1.326461000 | 1.705114000  |
| H | -7.609697000 | -1.913445000 | 0.668916000  |
| H | 0.619457000  | -6.364272000 | 2.259708000  |
| H | 0.027470000  | -7.797676000 | 1.425187000  |
| H | 6.710195000  | -1.879980000 | 0.123281000  |
| H | 7.400053000  | -2.390240000 | -1.414191000 |
| H | 2.719174000  | 5.236964000  | 2.958282000  |
| H | 5.329421000  | 3.637781000  | 0.727619000  |
| H | 7.045270000  | 0.114952000  | -1.364717000 |
| H | 5.207269000  | -3.072821000 | -2.269269000 |
| H | 2.161851000  | -6.961852000 | 0.375297000  |
| H | -6.490714000 | -1.003777000 | -1.338486000 |
| H | -5.886253000 | -3.701596000 | 1.310242000  |
| H | -1.667266000 | -6.554907000 | 0.237632000  |
| H | -1.414346000 | 6.147736000  | -0.568504000 |
| H | -4.977501000 | 4.342245000  | -2.250559000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -2.565722000 | 2.286394000  | 0.411119000  |
| H | 3.150903000  | -0.514693000 | -0.162850000 |

**IX[Cl<sup>-</sup>](M06-2X)**

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.588068000 | 4.117668000  | 0.839415000  |
| H | -0.278885000 | 3.075595000  | 0.884378000  |
| C | 0.469141000  | 5.094937000  | 1.084481000  |
| C | 1.787015000  | 4.791683000  | 0.768144000  |
| N | 2.107493000  | 3.613910000  | 0.161572000  |
| H | 1.355184000  | 2.944664000  | -0.053606000 |
| C | 3.389829000  | 3.139115000  | -0.141716000 |
| C | 4.557670000  | 4.012620000  | 0.255144000  |
| H | 5.406471000  | 3.377085000  | 0.518467000  |
| C | 4.200372000  | 4.957136000  | 1.406877000  |
| C | 2.928423000  | 5.735394000  | 1.056717000  |
| H | 3.117965000  | 6.350180000  | 0.164506000  |
| C | 3.483498000  | 1.934004000  | -0.755073000 |
| H | 2.542608000  | 1.421834000  | -0.960048000 |
| C | 4.714674000  | 1.256026000  | -1.171452000 |
| C | 5.787681000  | 2.011865000  | -1.728083000 |
| N | 6.657701000  | 2.644498000  | -2.184453000 |
| C | 4.871912000  | -0.113832000 | -1.101143000 |
| N | 3.879834000  | -0.908562000 | -0.576797000 |
| C | 3.921756000  | -2.284524000 | -0.353087000 |
| C | 5.201836000  | -2.977474000 | -0.760318000 |
| H | 5.899200000  | -3.004030000 | 0.088419000  |
| C | 5.870129000  | -2.261609000 | -1.937508000 |
| C | 6.133592000  | -0.804755000 | -1.561965000 |
| C | 2.818991000  | -2.886797000 | 0.179476000  |
| H | 1.917218000  | -2.292625000 | 0.303675000  |
| C | 2.680752000  | -4.261339000 | 0.612622000  |
| C | 3.838552000  | -5.060047000 | 0.886035000  |
| N | 4.765844000  | -5.722782000 | 1.135310000  |
| C | 1.446058000  | -4.859474000 | 0.862017000  |
| N | 0.331146000  | -4.113690000 | 0.607455000  |
| C | -0.882844000 | -4.614995000 | 0.721598000  |
| C | -1.145526000 | -6.013052000 | 1.253498000  |
| H | -2.076538000 | -6.027333000 | 1.824562000  |
| C | 0.026168000  | -6.489178000 | 2.115730000  |
| C | 1.337973000  | -6.290943000 | 1.355244000  |
| H | 1.362316000  | -6.972246000 | 0.491067000  |
| C | -1.934330000 | -3.721038000 | 0.316259000  |
| H | -1.617884000 | -2.696811000 | 0.138774000  |
| C | -3.263960000 | -3.981869000 | 0.068665000  |
| C | -3.810016000 | -5.307376000 | 0.131147000  |
| N | -4.296942000 | -6.366452000 | 0.155446000  |
| C | -4.207686000 | -2.922214000 | -0.325936000 |
| N | -3.802556000 | -1.690983000 | -0.207646000 |
| C | -4.613085000 | -0.616041000 | -0.507897000 |
| C | -5.996275000 | -0.840083000 | -1.095959000 |
| H | -6.754990000 | -0.782940000 | -0.303177000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | -6.087538000 | -2.204071000 | -1.787074000 |
| C  | -5.581612000 | -3.302349000 | -0.849583000 |
| H  | -5.544754000 | -4.270285000 | -1.358335000 |
| C  | -4.066045000 | 0.611246000  | -0.207544000 |
| H  | -3.039475000 | 0.551513000  | 0.147614000  |
| C  | -4.670083000 | 1.917277000  | -0.262185000 |
| C  | -6.076654000 | 2.063733000  | -0.465602000 |
| N  | -7.226359000 | 2.215678000  | -0.606897000 |
| C  | -3.973413000 | 3.117161000  | -0.015202000 |
| N  | -2.645159000 | 3.167306000  | 0.205666000  |
| C  | -1.877686000 | 4.322502000  | 0.494994000  |
| C  | -2.555027000 | 5.664754000  | 0.359348000  |
| H  | -2.822265000 | 6.048380000  | 1.353340000  |
| C  | -3.815131000 | 5.576627000  | -0.500829000 |
| C  | -4.702578000 | 4.442701000  | 0.016403000  |
| H  | -5.000576000 | 4.656633000  | 1.053519000  |
| C  | 0.186302000  | 6.356917000  | 1.676108000  |
| N  | -0.059936000 | 7.386211000  | 2.173479000  |
| H  | 6.568169000  | -0.243203000 | -2.392103000 |
| H  | 5.027890000  | 5.648498000  | 1.596259000  |
| H  | 4.038658000  | 4.386016000  | 2.329166000  |
| H  | -3.550500000 | 5.385420000  | -1.547813000 |
| H  | -4.361496000 | 6.524727000  | -0.473776000 |
| H  | -7.118226000 | -2.404484000 | -2.098229000 |
| H  | -5.472908000 | -2.198548000 | -2.695977000 |
| H  | 0.052611000  | -5.911172000 | 3.047830000  |
| H  | -0.105708000 | -7.539987000 | 2.392994000  |
| H  | 6.809214000  | -2.761590000 | -2.194617000 |
| H  | 5.223688000  | -2.311247000 | -2.821917000 |
| H  | 2.639821000  | 6.422709000  | 1.854442000  |
| H  | 4.883477000  | 4.605479000  | -0.610369000 |
| H  | 6.873240000  | -0.772526000 | -0.748606000 |
| H  | 4.989693000  | -4.015821000 | -1.012709000 |
| H  | 2.200376000  | -6.552560000 | 1.973945000  |
| H  | -6.243598000 | -0.044413000 | -1.800981000 |
| H  | -6.278124000 | -3.428683000 | -0.007161000 |
| H  | -1.300281000 | -6.704709000 | 0.414075000  |
| H  | -1.840816000 | 6.382147000  | -0.053245000 |
| H  | -5.626638000 | 4.363310000  | -0.557065000 |
| H  | -2.077342000 | 2.317910000  | 0.095182000  |
| H  | 3.025032000  | -0.440545000 | -0.285777000 |
| Cl | 0.039981000  | 0.975998000  | -0.275266000 |

**X (M06-2X)**

|   |              |             |              |
|---|--------------|-------------|--------------|
| C | -0.795238000 | 3.940758000 | -0.640887000 |
| H | -0.603501000 | 2.916304000 | -0.970736000 |
| C | 0.171660000  | 4.950455000 | -1.100216000 |
| C | 1.530762000  | 4.716446000 | -1.085963000 |
| N | 2.010998000  | 3.574981000 | -0.496511000 |
| H | 1.327563000  | 3.025932000 | 0.009022000  |
| C | 3.328683000  | 3.108742000 | -0.452896000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | 4.366153000  | 3.991399000  | -1.103179000 |
| H | 4.819319000  | 4.637241000  | -0.339108000 |
| C | 3.762246000  | 4.860868000  | -2.214097000 |
| C | 2.558690000  | 5.646043000  | -1.676700000 |
| H | 2.093920000  | 6.258035000  | -2.452375000 |
| C | 3.575314000  | 1.929129000  | 0.170848000  |
| H | 2.712587000  | 1.390773000  | 0.570862000  |
| C | 4.880159000  | 1.347664000  | 0.504535000  |
| C | 5.949797000  | 2.214223000  | 0.876725000  |
| N | 6.806067000  | 2.949463000  | 1.174159000  |
| C | 5.077614000  | -0.015003000 | 0.596684000  |
| N | 4.104046000  | -0.880279000 | 0.161084000  |
| C | 4.025134000  | -2.262028000 | 0.374098000  |
| C | 5.116865000  | -2.874818000 | 1.225331000  |
| H | 4.679824000  | -3.654192000 | 1.854483000  |
| C | 5.867924000  | -1.842888000 | 2.074002000  |
| C | 6.297025000  | -0.656979000 | 1.198776000  |
| C | 3.000054000  | -2.953298000 | -0.187481000 |
| H | 2.295295000  | -2.380531000 | -0.794878000 |
| C | 2.777605000  | -4.404011000 | -0.139036000 |
| C | 3.903563000  | -5.279100000 | -0.154281000 |
| N | 4.837062000  | -5.979489000 | -0.175104000 |
| C | 1.522991000  | -4.983233000 | -0.161039000 |
| N | 0.394529000  | -4.200828000 | -0.150620000 |
| C | -0.941587000 | -4.603326000 | -0.306373000 |
| C | -1.168381000 | -6.089945000 | -0.207332000 |
| H | -1.235584000 | -6.357602000 | 0.857502000  |
| C | -0.010089000 | -6.866835000 | -0.845425000 |
| C | 1.312012000  | -6.478487000 | -0.177928000 |
| H | 2.164054000  | -6.959064000 | -0.662937000 |
| C | -1.883495000 | -3.644808000 | -0.499337000 |
| H | -1.517174000 | -2.616105000 | -0.524821000 |
| C | -3.321288000 | -3.784228000 | -0.758127000 |
| C | -3.815723000 | -4.926962000 | -1.453781000 |
| N | -4.215622000 | -5.860647000 | -2.028514000 |
| C | -4.235294000 | -2.795893000 | -0.448179000 |
| N | -3.847837000 | -1.684052000 | 0.261709000  |
| C | -4.554571000 | -0.487600000 | 0.434303000  |
| C | -5.993447000 | -0.492612000 | -0.017780000 |
| H | -6.631034000 | -0.790317000 | 0.825809000  |
| C | -6.218044000 | -1.451655000 | -1.193007000 |
| C | -5.689558000 | -2.848408000 | -0.843131000 |
| H | -5.821244000 | -3.545654000 | -1.671913000 |
| C | -3.925078000 | 0.575950000  | 0.989519000  |
| H | -2.870856000 | 0.458873000  | 1.254589000  |
| C | -4.542363000 | 1.865174000  | 1.351292000  |
| C | -5.776698000 | 1.864901000  | 2.062830000  |
| N | -6.792341000 | 1.829568000  | 2.637355000  |
| C | -3.928336000 | 3.068276000  | 1.078824000  |
| N | -2.783535000 | 3.083380000  | 0.322476000  |
| C | -1.926795000 | 4.159693000  | 0.072770000  |
| C | -2.359253000 | 5.496511000  | 0.625044000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| H | -1.471919000 | 6.092544000  | 0.850068000  |
| C | -3.255764000 | 5.347255000  | 1.861408000  |
| C | -4.428669000 | 4.406685000  | 1.554576000  |
| H | -5.075217000 | 4.267666000  | 2.423248000  |
| C | -0.308885000 | 6.174661000  | -1.647593000 |
| N | -0.733702000 | 7.170257000  | -2.084890000 |
| H | 6.952520000  | -1.019808000 | 0.394388000  |
| H | 3.447479000  | 4.233350000  | -3.056501000 |
| H | 4.519191000  | 5.552182000  | -2.594812000 |
| H | -3.632618000 | 6.327795000  | 2.165348000  |
| H | -2.676059000 | 4.950755000  | 2.703537000  |
| H | -7.284193000 | -1.505504000 | -1.430460000 |
| H | -5.707674000 | -1.077495000 | -2.088586000 |
| H | -0.177409000 | -7.942233000 | -0.738426000 |
| H | 0.031108000  | -6.654137000 | -1.919960000 |
| H | 5.233716000  | -1.480680000 | 2.891813000  |
| H | 6.743549000  | -2.312385000 | 2.530953000  |
| H | 2.899919000  | 6.336718000  | -0.892303000 |
| H | 5.176381000  | 3.368013000  | -1.487960000 |
| H | 6.862384000  | 0.083697000  | 1.766462000  |
| H | 5.828882000  | -3.390085000 | 0.568681000  |
| H | 1.307647000  | -6.835406000 | 0.862147000  |
| H | -6.288663000 | 0.526313000  | -0.276732000 |
| H | -6.266337000 | -3.248615000 | 0.003142000  |
| H | -2.117852000 | -6.364326000 | -0.663195000 |
| H | -2.901953000 | 6.045461000  | -0.156361000 |
| H | -5.049932000 | 4.851402000  | 0.764147000  |
| H | -2.526285000 | 2.197830000  | -0.095325000 |
| H | 3.358372000  | -0.466964000 | -0.384152000 |
| H | 0.551107000  | -3.203478000 | -0.099048000 |
| H | -2.912885000 | -1.700644000 | 0.645452000  |

**X[Cl<sup>-</sup>](M06-2X)**

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.708300000 | 4.121014000  | -0.133993000 |
| H | -0.444490000 | 3.152372000  | -0.555588000 |
| C | 0.316676000  | 5.154935000  | -0.224223000 |
| C | 1.659473000  | 4.848060000  | -0.405639000 |
| N | 2.100724000  | 3.559518000  | -0.439771000 |
| H | 1.428562000  | 2.801471000  | -0.293209000 |
| C | 3.425077000  | 3.124579000  | -0.614169000 |
| C | 4.509292000  | 4.178332000  | -0.571853000 |
| H | 5.379247000  | 3.773305000  | -0.048587000 |
| C | 4.028370000  | 5.475623000  | 0.081321000  |
| C | 2.714257000  | 5.915078000  | -0.570204000 |
| H | 2.885163000  | 6.091714000  | -1.642598000 |
| C | 3.624909000  | 1.796020000  | -0.782413000 |
| H | 2.723052000  | 1.183842000  | -0.808234000 |
| C | 4.894756000  | 1.084181000  | -0.926438000 |
| C | 6.008364000  | 1.700129000  | -1.566794000 |
| N | 6.913206000  | 2.208767000  | -2.103868000 |
| C | 5.038798000  | -0.226022000 | -0.505717000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| N | 4.010978000  | -0.867628000 | 0.133097000  |
| C | 3.933273000  | -2.223897000 | 0.463952000  |
| C | 5.160660000  | -3.060722000 | 0.195448000  |
| H | 5.780551000  | -3.099604000 | 1.101923000  |
| C | 5.991963000  | -2.498442000 | -0.962313000 |
| C | 6.305293000  | -1.021390000 | -0.701882000 |
| C | 2.779800000  | -2.696965000 | 0.991239000  |
| H | 1.959459000  | -1.986801000 | 1.116315000  |
| C | 2.519308000  | -4.086256000 | 1.404420000  |
| C | 3.465595000  | -4.782581000 | 2.207015000  |
| N | 4.259661000  | -5.337203000 | 2.861487000  |
| C | 1.341270000  | -4.718543000 | 1.063009000  |
| N | 0.450076000  | -4.083421000 | 0.242277000  |
| C | -0.854711000 | -4.475722000 | -0.074063000 |
| C | -1.291458000 | -5.824197000 | 0.443803000  |
| H | -2.374045000 | -5.813497000 | 0.589743000  |
| C | -0.560005000 | -6.202105000 | 1.738110000  |
| C | 0.956266000  | -6.098312000 | 1.531920000  |
| H | 1.265277000  | -6.830392000 | 0.771537000  |
| C | -1.621923000 | -3.637327000 | -0.807714000 |
| H | -1.181281000 | -2.679417000 | -1.093798000 |
| C | -3.001670000 | -3.880911000 | -1.256781000 |
| C | -3.345901000 | -5.121983000 | -1.857585000 |
| N | -3.606380000 | -6.154121000 | -2.341718000 |
| C | -3.968946000 | -2.899554000 | -1.138360000 |
| N | -3.670091000 | -1.725924000 | -0.513191000 |
| C | -4.493439000 | -0.603392000 | -0.338318000 |
| C | -5.885549000 | -0.703068000 | -0.913491000 |
| H | -6.588015000 | -1.025937000 | -0.132963000 |
| C | -5.944956000 | -1.688376000 | -2.087255000 |
| C | -5.376813000 | -3.046015000 | -1.658532000 |
| H | -5.387008000 | -3.769851000 | -2.476473000 |
| C | -3.982473000 | 0.461477000  | 0.323097000  |
| H | -2.938862000 | 0.390731000  | 0.636361000  |
| C | -4.685532000 | 1.690112000  | 0.697817000  |
| C | -6.050484000 | 1.628615000  | 1.092666000  |
| N | -7.172015000 | 1.553836000  | 1.415751000  |
| C | -4.038484000 | 2.915965000  | 0.758924000  |
| N | -2.742148000 | 3.043901000  | 0.369365000  |
| C | -1.940202000 | 4.199220000  | 0.422665000  |
| C | -2.536568000 | 5.409219000  | 1.105819000  |
| H | -1.752327000 | 5.928320000  | 1.661389000  |
| C | -3.703282000 | 5.039373000  | 2.026506000  |
| C | -4.707583000 | 4.170644000  | 1.261470000  |
| H | -5.568652000 | 3.902946000  | 1.876806000  |
| C | -0.043512000 | 6.533102000  | -0.222373000 |
| N | -0.348488000 | 7.661728000  | -0.233715000 |
| H | 6.888807000  | -0.582296000 | -1.513182000 |
| H | 4.788109000  | 6.255920000  | -0.029810000 |
| H | 3.871782000  | 5.327231000  | 1.156694000  |
| H | -4.190330000 | 5.947838000  | 2.395013000  |
| H | -3.338829000 | 4.489637000  | 2.902641000  |



|    |              |              |              |
|----|--------------|--------------|--------------|
| H  | -6.979248000 | -1.803685000 | -2.426475000 |
| H  | -5.368349000 | -1.299869000 | -2.935375000 |
| H  | -0.866595000 | -5.533717000 | 2.551758000  |
| H  | -0.830488000 | -7.219560000 | 2.037709000  |
| H  | 6.920270000  | -3.068569000 | -1.069919000 |
| H  | 5.440700000  | -2.596932000 | -1.905357000 |
| H  | 2.348295000  | 6.855845000  | -0.154997000 |
| H  | 4.851172000  | 4.394042000  | -1.592674000 |
| H  | 6.919290000  | -0.942066000 | 0.207486000  |
| H  | 4.851117000  | -4.089483000 | -0.002554000 |
| H  | 1.508341000  | -6.339441000 | 2.442767000  |
| H  | -6.215483000 | 0.292386000  | -1.219128000 |
| H  | -6.008027000 | -3.464282000 | -0.861076000 |
| H  | -1.095727000 | -6.588643000 | -0.320950000 |
| H  | -2.887388000 | 6.124672000  | 0.350307000  |
| H  | -5.095007000 | 4.740012000  | 0.403894000  |
| H  | -2.265866000 | 2.214716000  | 0.022121000  |
| H  | 3.152465000  | -0.341535000 | 0.280367000  |
| H  | 0.726895000  | -3.167073000 | -0.094821000 |
| H  | -2.731426000 | -1.637820000 | -0.138707000 |
| Cl | 0.251660000  | 0.472257000  | -0.056663000 |