Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics


# Supporting Information

## Contrasting Preferences of N and P Substituted Heteroaromatics Towards Metal Binding: Probing the Regioselectivity of $Li^+$ and $Mg^{2+}$ Binding to $(CH)_{6-m-n}N_mP_n$

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Table S1: BSSE corrected binding energy (kcal/mol) of all the possible cation-π complexes with $Li^+$ and $Mg^{2+}$ at CCSD(T)/cc-pVTZ level and the corresponding NICS (1) values at B3LYP/cc-pVTZ level.

| Name | $Li^+$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | B.E | NICS (1) | B.E | NICS (1) |
| **Ben-π** | 36.60 | -8.17 | 114.44 | -3.92 |
| **1N–π** | 28.24 | -6.81 | 97.29 | -2.48 |
| **3N–π** | 19.38 | -5.14 | 78.97 | -1.45 |
| **4N–π** | 19.31 | -4.96 | 79.45 | -1.25 |
| **7N–π** | 9.78 | -3.31 | 57.58 | -0.31 |
| **1P–π** | 34.61 | -7.14 | 114.85 | -2.62 |
| **2P–π** | 30.28 | -6.31 | 107.60 | -2.49 |
| **3P–π** | 31.46 | -5.77 | 113.67 | -1.40 |
| **4P–π** | 31.18 | -5.80 | 115.34 | -1.28 |
| **5P–π** | 27.72 | -5.70 | 113.04 | -2.21 |
| **6P–π** | 28.92 | -5.33 | 116.14 | -1.85 |
| **7P–π** | 29.91 | -4.65 | 119.49 | -0.24 |
| **8P–π** | 25.99 | -5.86 | 114.43 | -3.67 |
| **9P–π** | 26.94 | -5.05 | 117.01 | -1.84 |
| **10P–π** | 28.41 | -7.08 | 119.11 | -5.18 |
| **11P–π** | 25.50 | -10.67 | 117.35 | -8.79 |
| **13–π** | 26.54 | -5.07 | 101.06 | -0.70 |
| **14–π** | 26.02 | -5.50 | 99.00 | -1.54 |
| **15–π** | 25.92 | -5.23 | 98.09 | -1.21 |
| **18N–π** | 18.67 | -3.30 | 86.35 | 0.04 |
| **19N–π** | 18.63 | -3.33 | 85.07 | -0.99 |
| **20N–π** | 18.49 | -4.21 | 83.89 | -1.49 |
| **21N–π** | 18.83 | -3.33 | 86.48 | 0.00 |
| **32–π** | 18.48 | -1.48 | 95.67 | -2.40 |
| **33-–π** | 18.76 | -2.87 | 93.49 | -2.07 |
| **34–π** | 19.40 | -6.17 | 91.63 | -6.82 |
| **35–π** | -a- | -a- | 99.72 | -6.46 |
| **36–π** | 19.04 | -3.08 | 96.51 | -3.46 |
| **37–π** | 19.40 | -1.49 | 95.62 | 0.22 |
| **38–π** | 20.91 | -6.82 | 94.34 | -3.49 |
| **16P–π** | 24.17 | -4.45 | 100.07 | -1.40 |
| **17P–π** | 23.36 | -4.54 | 98.10 | -1.40 |
| **18P–π** | 25.77 | -2.88 | 106.30 | 1.56 |
| **19P–π** | 24.80 | -3.79 | 103.08 | 0.34 |
| **20P–π** | 24.74 | -4.53 | 103.03 | -1.19 |
| **21P–π** | 24.92 | -3.85 | -a- | -a- |
| **23P–π** | 21.52 | -4.25 | -a- | -a- |
| **24P–π** | 24.54 | -2.90 | 99.14 | -0.71 |
| **25P–π** | 22.51 | -4.64 | 109.49 | -3.46 |
| **26P–π** | 23.72 | -5.23 | 105.70 | -4.14 |
| **27P–π** | 24.46 | -1.77 | 109.46 | 2.98 |
| **39P–π** | 22.04 | -13.34 | 114.90 | -13.32 |
| **40P–π** | 22.72 | -9.18 | 116.50 | -13.64 |
| **41P–π** | 26.52 | -10.20 | 114.47 | -9.13 |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S2: BSSE corrected binding energy (kcal/mol) of stable σ-complexes with $Li^{+}$ and $Mg^{2+}$ at CCSD(T)/cc-pVTZ level and the corresponding NICS (1) B3LYP/cc-pVTZ level.

| Name | $Li^{+}$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | B.E | NICS (1) | B.E | NICS (1) |
| **1N–σ′$_{1N}$** | 44.50 | -9.82 | 122.21 | -9.30 |
| **2N–σ″$_{1N}$** | 54.06 | -10.12 | 144.23 | -9.66 |
| **3N–σ′$_{1N}$** | 38.86 | -9.47 | 110.68 | -8.56 |
| **4N–σ′$_{1N}$** | 36.98 | -9.95 | 105.55 | -9.55 |
| **5N–σ″$_{2N}$** | 47.30 | -10.33 | 130.60 | -9.87 |
| **6N–σ″$_{1N}$** | 45.67 | -9.92 | 126.92 | -9.22 |
| **7N–σ′$_{1N}$** | 32.72 | -8.93 | -a- | -a- |
| **8N–σ″$_{3N}$** | 40.46 | -10.33 | 116.28 | -9.88 |
| **9N–σ″$_{2N}$** | 38.17 | -9.87 | 111.53 | -9.19 |
| **10N–σ″$_{1N}$** | 35.56 | -10.26 | 106.02 | -9.29 |
| **11N–σ″$_{2N}$** | -a- | -a- | 89.70 | -9.14 |
| **11N–σ′$_{3aN}$** | 30.66 | -9.88 | -a- | -a- |
| **13–σ′$_{2aN}$** | 43.87 | -8.91 | 127.62 | -8.73 |
| **14–σ′$_{1N}$** | 40.97 | -9.32 | 117.77 | -8.62 |
| **15–σ′$_{1N}$** | 41.98 | -9.10 | 120.16 | -8.34 |
| **16N–σ″$_{2N}$** | 53.37 | -9.13 | 146.98 | -8.62 |
| **17N– σ″$_{1N}$** | 51.89 | -9.41 | 143.05 | -8.88 |
| **18N–σ′$_{2aN}$** | 38.92 | -8.09 | 116.44 | -7.31 |
| **19N–σ′$_{1N}$** | 38.11 | -8.18 | 112.95 | -6.82 |
| **20N–σ′$_{1N}$** | 35.86 | -8.94 | 107.36 | -6.72 |
| **21N–σ′$_{2aN}$** | 36.97 | -8.81 | 112.70 | -7.57 |
| **22N–σ″$_{3N}$** | 47.62 | -9.09 | 135.37 | -8.59 |
| **23N– σ″$_{2N}$** | 46.20 | -9.49 | 131.81 | -8.81 |
| **24N–σ″$_{2N}$** | 46.87 | -8.36 | 134.12 | -7.41 |
| **25N–σ″$_{2N}$** | 46.07 | -8.79 | 131.74 | -7.86 |
| **26N–σ″$_{1N}$** | 46.08 | -8.52 | 131.57 | -7.35 |
| **27N– σ′$_{1N}$** | 33.83 | -7.14 | 105.32 | -5.18 |
| **28– σ″$_{2N}$** | 49.95 | -8.61 | 143.09 | -8.04 |
| **29– σ″$_{2N}$** | 51.53 | -8.37 | 146.10 | -7.76 |
| **30– σ″$_{3N}$** | 52.44 | -8.07 | 148.70 | -7.57 |
| **31– σ″$_{1N}$** | 49.38 | -8.79 | 140.43 | -8.30 |
| **32– σ′$_{3bN}$** | 38.61 | -6.73 | 121.16 | -5.52 |
| **33– σ′$_{2aN}$** | 35.92 | -7.42 | 112.28 | -6.45 |
| **34– σ′$_{2aN}$** | 35.82 | -7.91 | -a- | -a- |
| **35–σ′$_{2aN}$** | 38.27 | -7.00 | 118.53 | -5.05 |
| **36–σ′$_{2aN}$** | 36.31 | -7.78 | 125.28 | -6.43 |
| **37– σ′$_{3aN}$** | 36.80 | -7.35 | 115.10 | -6.19 |
| **38–σ′$_{2aN}$** | 35.40 | -7.48 | 115.01 | -5.11 |
| **39N–σ″$_{3N}$** | 41.54 | -8.64 | 122.70 | -7.91 |
| **40N–σ″$_{3N}$** | 40.75 | -7.94 | 121.78 | -6.84 |
| **41N– σ″$_{2N}$** | 37.90 | 8.66 | -a- | -a- |
| **42N– σ″$_{3N}$** | 45.17 | -8.29 | 133.75 | -7.53 |
| **43N– σ″$_{3N}$** | 47.12 | -7.67 | 138.36 | -7.01 |
| **44N– σ″$_{2N}$** | 45.31 | -7.38 | -a- | -a- |
| **45N– σ″$_{2N}$** | 47.29 | 6.61 | 138.74 | -5.09 |
| **46N– σ″$_{3N}$** | 46.77 | -7.08 | -a- | -a- |
| **47N– σ′$_{2aN}$** | 34.49 | -5.26 | 111.36 | -2.12 |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S3: BSSE corrected binding energy of stable σ-complexes with $Li^{+}$ and $Mg^{2+}$ at CCSD(T)/cc-pVTZ level and the corresponding NICS (1) values at B3LYP/cc-pVTZ level

| Name | $Li^{+}$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | B.E | NICS (1) | B.E | NICS (1) |
| **1P–σ′$_{1P}$** | 31.48 | -9.64 | -a- | -a- |
| **2P–σ′$_{2aP}$** | 31.79 | -9.31 | -a- | -a- |
| **3P–σ′$_{1P}$** | 29.28 | -9.10 | -a- | -a- |
| **4P–σ′$_{1P}$** | 29.28 | -9.00 | -a- | -a- |
| **5P–σ′$_{3aP}$** | 32.34 | -8.97 | 125.87 | -8.59 |
| **6P–σ′$_{2aP}$** | 29.96 | -8.77 | -a- | -a- |
| **7P–σ′$_{1P}$** | 27.52 | -8.58 | -a- | -a- |
| **8P–σ′$_{3bP}$** | 30.53 | -8.80 | 125.29 | -8.02 |
| **9P–σ′$_{3aP}$** | 31.36 | -8.47 | 128.30 | -7.73 |
| **10P–σ′$_{2aP}$** | 28.20 | -8.52 | 118.53 | -7.16 |
| **11P–σ′$_{3aP}$** | 28.83 | -9.09 | -a- | -a- |
| **16P–σ′$_{2aN}$** | 40.83 | -8.63 | 114.91 | -8.59 |
| **17P–σ′$_{1N}$** | 38.26 | -8.71 | 112.66 | -7.40 |
| **18P–σ′$_{3aN}$** | 43.12 | -7.72 | -a- | -a- |
| **19P–σ′$_{2aN}$** | 41.80 | -8.18 | 127.80 | -7.83 |
| **20P–σ′$_{1N}$** | 38.13 | -8.76 | 114.38 | -6.77 |
| **21P–σ′$_{2aN}$** | 40.44 | -8.34 | 124.59 | -8.10 |
| **22P–σ′$_{2aN}$** | 38.67 | -8.21 | 130.09 | -8.01 |
| **23P–σ′$_{1N}$** | 35.15 | -8.37 | 110.44 | -3.29 |
| **24P–σ′$_{3bN}$** | 40.04 | -7.43 | 131.71 | -7.23 |
| **25P–σ′$_{2aN}$** | 38.10 | -8.14 | 128.61 | -8.01 |
| **26P–σ′$_{2aN}$** | 37.98 | -7.83 | 123.80 | -7.80 |
| **27P– σ′$_{3aN}$** | 41.37 | -6.99 | -a- | -a- |
| **39P– σ′$_{2aN}$** | 35.46 | -8.30 | 127.28 | -8.56 |
| **40P– σ′$_{3bN}$** | 38.05 | -7.13 | 131.99 | -6.71 |
| **41P–σ′$_{3aN}$** | 37.29 | -7.33 | -a- | -a- |
| **42P– σ″$_{2N}$** | 47.69 | -8.12 | 141.01 | -7.60 |
| **44P– σ″$_{3N}$** | 49.32 | -7.62 | 145.22 | -7.03 |
| **45P– σ′$_{2aN}$** | 34.79 | -5.97 | 114.76 | -4.94 |
| **46P– σ′$_{2aN}$** | 35.75 | -6.18 | -a- | -a- |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S4: NPA and Mulliken charge (au) on metal ions for the cation-π complexes MP2/cc-pVTZ level.

| Complexes | $Li^+$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | NPA | Mulliken | NPA | Mulliken |
| **1N–π** | 0.910 | 0.483 | 1.809 | 1.087 |
| **3N–π** | 0.924 | 0.555 | 1.837 | 1.167 |
| **4N–π** | 0.920 | 0.533 | 1.830 | 1.146 |
| **7N–π** | 0.941 | 0.628 | 1.855 | 1.207 |
| **1P–π** | 0.861 | 0.410 | 1.703 | 0.946 |
| **2P–π** | 0.829 | 0.406 | 1.616 | 0.885 |
| **3P–π** | 0.826 | 0.404 | 1.640 | 0.893 |
| **4P–π** | 0.819 | 0.406 | 1.644 | 0.892 |
| **5P–π** | 0.794 | 0.399 | 1.527 | 0.827 |
| **6P–π** | 0.790 | 0.402 | 1.569 | 0.838 |
| **7P–π** | 0.783 | 0.400 | 1.573 | 0.842 |
| **8P–π** | 0.758 | 0.392 | 1.457 | 0.774 |
| **9P–π** | 0.751 | 0.396 | 1.471 | 0.780 |
| **10P–π** | 0.766 | 0.397 | 1.535 | 0.804 |
| **11P–π** | 0.734 | 0.388 | 1.408 | 0.738 |
| **13–π** | 0.873 | 0.461 | 1.731 | 1.017 |
| **14–π** | 0.882 | 0.466 | 1.740 | 1.014 |
| **15–π** | 0.888 | 0.470 | 1.742 | 1.017 |
| **18N–π** | 0.885 | 0.511 | 1.758 | 1.087 |
| **19N–π** | 0.902 | 0.536 | 1.787 | 1.119 |
| **20N–π** | 0.900 | 0.524 | 1.783 | 1.088 |
| **21N–π** | 0.890 | 0.511 | 1.764 | 1.076 |
| **32–π** | 0.854 | 0.498 | 1.729 | 1.071 |
| **33—π** | 0.852 | 0.487 | 1.728 | 1.029 |
| **34–π** | 0.896 | 0.526 | 1.764 | 1.075 |
| **35–π** | -a- | -a- | 1.806 | 1.133 |
| **36–π** | 0.861 | 0.485 | 1.714 | 1.029 |
| **37–π** | 0.863 | 0.494 | 1.714 | 1.028 |
| **38–π** | 0.854 | 0.465 | 1.734 | 1.009 |
| **16P–π** | 0.848 | 0.448 | 1.656 | 0.954 |
| **17P–π** | 0.861 | 0.455 | 1.660 | 0.949 |
| **18P–π** | 0.831 | 0.446 | 1.665 | 0.963 |
| **19P–π** | 0.846 | 0.450 | 1.670 | 0.953 |
| **20P–π** | 0.853 | 0.453 | 1.685 | 0.957 |
| **21P–π** | 0.838 | 0.449 | -a- | -a- |
| **23P–π** | 0.836 | 0.448 | -a- | -a- |
| **24P–π** | 0.797 | 0.434 | 1.609 | 0.914 |
| **25P–π** | 0.815 | 0.438 | 1.630 | 0.916 |
| **26P–π** | 0.817 | 0.432 | 1.631 | 0.900 |
| **27P–π** | 0.792 | 0.437 | 1.595 | 0.902 |
| **39P–π** | 0.805 | 0.427 | 1.543 | 0.890 |
| **40P–π** | 0.814 | 0.444 | 1.618 | 0.921 |
| **41P–π** | 0.799 | 0.423 | 1.613 | 0.897 |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S5: NPA and Mulliken charge (au) on metal ions for the cation-σ complexes, at MP2/cc-pVTZ level.

| Complexes | $Li^{+}$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | NPA | Mulliken | NPA | Mulliken |
| **1N–σ′$_{1N}$** | 0.960 | 0.644 | 1.872 | 1.331 |
| **2N–σ″$_{1N}$** | 0.924 | 0.544 | 1.866 | 1.311 |
| **3N–σ′$_{1N}$** | 0.960 | 0.661 | 1.870 | 1.356 |
| **4N–σ′$_{1N}$** | 0.963 | 0.667 | 1.833 | 1.379 |
| **5N–σ″$_{2N}$** | 0.932 | 0.614 | 1.865 | 1.364 |
| **6N–σ″$_{1N}$** | 0.932 | 0.598 | 1.878 | 1.355 |
| **7N–σ′$_{1N}$** | 0.961 | 0.680 | -a- | -a- |
| **8N–σ″$_{3N}$** | 0.938 | 0.648 | 1.864 | 1.404 |
| **9N–σ″$_{2N}$** | 0.940 | 0.650 | 1.879 | 1.411 |
| **10N–σ″$_{1N}$** | 0.939 | 0.636 | 1.890 | 1.404 |
| **11N–σ″$_{2N}$** | -a- | -a- | 1.896 | 1.464 |
| **11N–σ′$_{3aN}$** | 0.963 | 0.734 | -a- | -a- |
| **13–σ′$_{2aN}$** | 0.952 | 0.626 | 1.802 | 1.213 |
| **14–σ′$_{1N}$** | 0.958 | 0.646 | 1.859 | 1.323 |
| **15–σ′$_{1N}$** | 0.960 | 0.644 | 1.868 | 1.318 |
| **16N–σ″$_{2N}$** | 0.924 | 0.557 | 1.863 | 1.292 |
| **17N– σ″$_{1N}$** | 0.922 | 0.563 | 1.856 | 1.295 |
| **18N–σ′$_{2aN}$** | 0.955 | 0.648 | 1.842 | 1.323 |
| **19N–σ′$_{1N}$** | 0.958 | 0.656 | 1.858 | 1.329 |
| **20N–σ′$_{1N}$** | 0.958 | 0.665 | 1.856 | 1.347 |
| **21N–σ′$_{2aN}$** | 0.958 | 0.652 | 1.817 | 1.259 |
| **22N–σ″$_{3N}$** | 0.931 | 0.601 | 1.861 | 1.336 |
| **23N– σ″$_{2N}$** | 0.930 | 0.609 | 1.854 | 1.342 |
| **24N–σ″$_{2N}$** | 0.929 | 0.581 | 1.871 | 1.322 |
| **25N–σ″$_{2N}$** | 0.930 | 0.586 | 1.107 | 1.328 |
| **26N–σ″$_{1N}$** | 0.927 | 0.587 | 1.865 | 1.327 |
| **27N– σ′$_{1N}$** | 0.958 | 0.668 | 1.864 | 1.362 |
| **28– σ″$_{2N}$** | 0.932 | 0.564 | 1.855 | 1.281 |
| **29– σ″$_{2N}$** | 0.936 | 0.557 | 1.854 | 1.278 |
| **30– σ″$_{3N}$** | 0.935 | 0.553 | 1.860 | 1.275 |
| **31– σ″$_{1N}$** | 0.924 | 0.566 | 1.849 | 1.286 |
| **32– σ′$_{3bN}$** | 0.922 | 0.649 | 1.851 | 1.328 |
| **33– σ′$_{2aN}$** | 0.924 | 0.652 | 1.783 | 1.264 |
| **34– σ′$_{2aN}$** | 0.921 | 0.651 | -a- | -a- |
| **35–σ′$_{2aN}$** | 0.953 | 0.643 | 1.808 | 1.232 |
| **36–σ′$_{2aN}$** | 0.952 | 0.628 | 1.765 | 1.167 |
| **37– σ′$_{3aN}$** | 0.955 | 0.652 | 1.868 | 1.341 |
| **38–σ′$_{2aN}$** | 0.955 | 0.649 | 1.786 | 1.217 |
| **39N–σ″$_{3N}$** | 0.943 | 0.638 | 1.749 | 1.368 |
| **40N–σ″$_{3N}$** | 0.955 | 0.625 | 1.775 | 1.368 |
| **41N– σ″$_{2N}$** | 0.954 | 0.614 | -a- | -a- |
| **42N– σ″$_{3N}$** | 0.931 | 0.605 | 1.852 | 1.319 |
| **43N– σ″$_{3N}$** | 0.927 | 0.597 | 1.842 | 1.311 |
| **44N– σ″$_{2N}$** | 0.928 | 0.583 | -a- | -a- |
| **45N– σ″$_{2N}$** | 0.924 | 0.573 | 1.859 | 1.298 |
| **46N– σ″$_{3N}$** | 0.927 | 0.573 | -a- | -a- |
| **47N– σ′$_{2aN}$** | 0.954 | 0.658 | 1.847 | 1.328 |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S6: NPA and Mulliken charge (au) on metal ions for the cation-σ complexes for the P-analogs at MP2/cc-pVTZ level.

| Complexes | $Li^+$ | | $Mg^{2+}$ | |
|---|---|---|---|---|
| | NPA | Mulliken | NPA | Mulliken |
| **1P–σ′$_{1P}$** | 0.915 | 0.642 | -a- | -a- |
| **2P–σ′$_{2aP}$** | 0.928 | 0.639 | -a- | -a- |
| **3P–σ′$_{1P}$** | 0.914 | 0.645 | -a- | -a- |
| **4P–σ′$_{1P}$** | 0.914 | 0.643 | -a- | -a- |
| **5P–σ′$_{3aP}$** | 0.940 | 0.639 | 1.682 | 1.118 |
| **6P–σ′$_{2aP}$** | 0.926 | 0.640 | -a- | -a- |
| **7P–σ′$_{1P}$** | 0.912 | 0.645 | -a- | -a- |
| **8P–σ′$_{3bP}$** | 0.938 | 0.644 | 1.638 | 1.105 |
| **9P–σ′$_{3aP}$** | 0.939 | 0.639 | 1.674 | 1.109 |
| **10P–σ′$_{2aP}$** | 0.926 | 0.641 | 1.642 | 1.118 |
| **11P–σ′$_{3aP}$** | 0.937 | 0.647 | -a- | -a- |
| **16P–σ′$_{2aN}$** | 0.943 | 0.615 | 1.785 | 1.168 |
| **17P–σ′$_{1N}$** | 0.959 | 0.650 | 1.313 | 1.313 |
| **18P–σ′$_{3aN}$** | 0.950 | 0.627 | -a- | -a- |
| **19P–σ′$_{2aN}$** | 0.949 | 0.624 | 1.781 | 1.179 |
| **20P–σ′$_{1N}$** | 0.957 | 0.648 | 1.845 | 1.316 |
| **21P–σ′$_{2aN}$** | 0.950 | 0.631 | 1.778 | 1.189 |
| **22P–σ′$_{2aN}$** | 0.939 | 0.614 | 1.776 | 1.141 |
| **23P–σ′$_{1N}$** | 0.958 | 0.655 | 1.848 | 1.312 |
| **24P–σ′$_{3bN}$** | 0.948 | 0.628 | 1.793 | 1.164 |
| **25P–σ′$_{2aN}$** | 0.939 | 0.614 | 1.767 | 1.148 |
| **26P–σ′$_{2aN}$** | 0.947 | 0.631 | 1.760 | 1.160 |
| **27P– σ′$_{3aN}$** | 0.947 | 0.624 | -a- | -a- |
| **39P– σ′$_{2aN}$** | 0.935 | 0.615 | 1.749 | 1.124 |
| **40P– σ′$_{3bN}$** | 0.944 | 0.624 | 1.775 | 1.138 |
| **41P–σ′$_{3aN}$** | 0.949 | 0.636 | -a- | -a- |
| **42P– σ′′$_{2N}$** | 0.923 | 0.569 | 1.850 | 1.276 |
| **44P– σ′′$_{3N}$** | 0.924 | 0.558 | 1.853 | 1.267 |
| **45P– σ′$_{2aN}$** | 0.948 | 0.651 | 1.749 | 1.217 |
| **46P– σ′$_{2aN}$** | 0.934 | 0.641 | -a- | -a- |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S7: Polarizability (ά) in au of the N and P substituted heteroaromatics at MP2/cc-pVTZ level

| N > P | | | P > N | | | P=N | |
|---|---|---|---|---|---|---|---|
| **Name** | **P, N** | **ά** | **Name** | **P, N** | **ά** | **Name** | **ά** |
| **1N** | N=1, P=0 | 57.40 | **1P** | P=1, N=0 | 74.85 | **13** | 69.75 |
| **2N** | N=2, P=0 | 52.71 | **2P** | P=2, N=0 | 88.48 | **14** | 70.21 |
| **3N** | N=2, P=0 | 52.58 | **3P** | P=2, N=0 | 88.00 | **15** | 69.80 |
| **4N** | N=2, P=0 | 52.97 | **4P** | P=2, N=0 | 88.29 | **28** | 69.75 |
| **5N** | N=3, P=0 | 48.35 | **5P** | P=3, N=0 | 102.95 | **29** | 70.21 |
| **6N** | N=3, P=0 | 48.34 | **6P** | P=3, N=0 | 102.20 | **30** | 69.80 |
| **7N** | N=3, P=0 | 47.58 | **7P** | P=3, N=0 | 101.42 | **31** | 78.77 |
| **8N** | N=4, P=0 | 44.02 | **8P** | P=4, N=0 | 117.69 | **32** | 77.57 |
| **9N** | N=4, P=0 | 43.98 | **9P** | P=4, N=0 | 116.98 | **33** | 77.24 |
| **10N** | N=4, P=0 | 44.22 | **10P** | P=4, N=0 | 116.57 | **34** | 78.51 |
| **11N** | N=4, P=0 | 40.17 | **11P** | P=4, N=0 | 133.05 | **35** | 76.16 |
| **16N** | N=2, P=1 | 64.77 | **16P** | P=2, N=1 | 64.77 | **36** | 78.65 |
| **17N** | N=2, P=1 | 65.13 | **17P** | P=2, N=1 | 83.64 | **37** | 78.78 |
| **18N** | N=2, P=1 | 64.28 | **18P** | P=2, N=1 | 82.30 | **38** | 76.52 |
| **19N** | N=2, P=1 | 64.46 | **19P** | P=2, N=1 | 82.48 | **52** | 78.96 |
| **20N** | N=2, P=1 | 65.57 | **20P** | P=2, N=1 | 83.19 | **53** | 76.16 |
| **21N** | N=2, P=1 | 65.22 | **21P** | P=2, N=1 | 83.36 | **54** | 77.94 |
| **22N** | N=3, P=1 | 60.16 | **22P** | P=3, N=1 | 97.90 | | |
| **23N** | N=3, P=1 | 60.55 | **23P** | P=3, N=1 | 97.94 | | |
| **24N** | N=3, P=1 | 59.61 | **24P** | P=3, N=1 | 97.30 | | |
| **25N** | N=3, P=1 | 60.33 | **25P** | P=3, N=1 | 97.24 | | |
| **26N** | N=3, P=1 | 60.40 | **26P** | P=3, N=1 | 97.16 | | |
| **27N** | N=3, P=1 | 0.00 | **27P** | P=3, N=1 | 95.23 | | |
| **39N** | N=4, P=1 | 55.69 | **39P** | P=4, N=1 | 112.81 | | |
| **40N** | N=4, P=1 | 55.13 | **40P** | P=4, N=1 | 111.79 | | |
| **41N** | N=4, P=1 | 55.38 | **41P** | P=4, N=1 | 111.64 | | |
| **42N** | N=3, P=2 | 74.02 | **42P** | P=3, N=2 | 92.88 | | |
| **43N** | N=3, P=2 | 72.42 | **43P** | P=3, N=2 | 92.81 | | |
| **44N** | N=3, P=2 | 74.30 | **44P** | P=3, N=2 | 91.67 | | |
| **45N** | N=3, P=2 | 72.04 | **45P** | P=3, N=2 | 92.02 | | |
| **46N** | N=3, P=2 | 72.29 | **46P** | P=3, N=2 | 91.89 | | |
| **47N** | N=3, P=2 | 69.29 | **47P** | P=3, N=2 | 87.97 | | |

Table S8: NICS (1) obtained at B3LYP/cc-pVTZ level for the cation–σ complexes and their corresponding parent analogues.

| Complex | Parent | $Li^+$ | $Mg^{2+}$ |
|---|---|---|---|
| | NICS (1) | NICS (1) | NICS (1) |
| **1N–σ′$_{1N}$** | -10.14 | -9.82 | -9.30 |
| **2N–σ′′$_{1N}$** | -11.16 | -10.12 | -9.66 |
| **3N–σ′$_{1N}$** | -11.27 | -9.47 | -8.56 |
| **4N–σ′$_{1N}$** | -11.14 | -9.95 | -9.55 |
| **5N–σ′′$_{2N}$** | -11.13 | -10.33 | -9.87 |
| **6N–σ′′$_{1N}$** | -10.89 | -9.92 | -9.22 |
| **7N–σ′$_{1N}$** | -11.00 | -8.93 | -a- |
| **8N–σ′′$_{3N}$** | -10.72 | -10.33 | -9.88 |
| **9N–σ′′$_{2N}$** | -10.84 | -9.87 | -9.19 |
| **10N–σ′′$_{1N}$** | -10.56 | -10.26 | -9.29 |
| **11N–σ′′$_{2N}$** | -10.37 | -a- | -9.14 |
| **11N–σ′$_{3aN}$** | -10.37 | -9.88 | -a- |
| **13–σ′$_{2aN}$** | -9.73 | -8.91 | -8.73 |
| **14–σ′$_{1N}$** | -10.26 | -9.32 | -8.62 |
| **15–σ′$_{1N}$** | -10.14 | -9.10 | -8.34 |
| **16N–σ′′$_{2N}$** | -9.35 | -9.13 | -8.62 |
| **17N– σ′′$_{1N}$** | -9.74 | -9.41 | -8.88 |
| **18N–σ′$_{2aN}$** | -9.29 | -8.09 | -7.31 |
| **19N–σ′$_{1N}$** | -9.73 | -8.18 | -6.82 |
| **20N–σ′$_{1N}$** | -10.34 | -8.94 | -6.72 |
| **21N–σ′$_{2aN}$** | -9.33 | -8.81 | -7.57 |
| **22N–σ′′$_{3N}$** | -9.28 | -9.09 | -8.59 |
| **23N– σ′′$_{2N}$** | -9.72 | -9.49 | -8.81 |
| **24N–σ′′$_{2N}$** | -8.75 | -8.36 | -7.41 |
| **25N–σ′′$_{2N}$** | 9.08 | -8.79 | -7.86 |
| **26N–σ′′$_{1N}$** | -9.09 | -8.52 | -7.35 |
| **27N– σ′$_{1N}$** | -9.12 | -7.14 | -5.18 |
| **28– σ′′$_{2N}$** | -8.54 | -8.61 | -8.04 |
| **29– σ′′$_{2N}$** | -6.47 | -8.37 | -7.76 |
| **30– σ′′$_{3N}$** | -8.23 | -8.07 | -7.57 |
| **31– σ′′$_{1N}$** | -8.94 | -8.79 | -8.30 |
| **32– σ′$_{3bN}$** | -7.96 | -6.73 | -5.52 |
| **33– σ′$_{2aN}$** | -8.25 | -7.42 | -6.45 |
| **34– σ′$_{2aN}$** | -9.31 | -7.91 | -a- |
| **35–σ′$_{2aN}$** | -8.52 | -7.00 | -5.05 |
| **36–σ′$_{2aN}$** | -8.10 | -7.78 | -6.43 |
| **37– σ′$_{3aN}$** | -7.57 | -7.35 | -6.19 |
| **38–σ′$_{2aN}$** | -4.10 | -7.48 | -5.11 |
| **39N–σ′′$_{3N}$** | -8.49 | -8.64 | -7.91 |
| **40N–σ′′$_{3N}$** | -8.49 | -7.94 | -6.84 |
| **41N– σ′′$_{2N}$** | -8.05 | 8.66 | -a- |
| **42N– σ′′$_{3N}$** | -8.34 | -8.29 | -7.53 |
| **43N– σ′′$_{3N}$** | -7.80 | -7.67 | -7.01 |
| **44N– σ′′$_{2N}$** | -7.62 | -7.38 | -a- |
| **45N– σ′′$_{2N}$** | -6.87 | 6.61 | -5.09 |
| **46N– σ′′$_{3N}$** | -6.57 | -7.08 | -a- |
| **47N– σ′$_{2aN}$** | -7.16 | -5.26 | -2.12 |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S9: NICS (1) obtained at B3LYP/cc-pVTZ level for the hetero-substituted P-analogs cation–σ complexes and their corresponding parent analogues.

| Complex | Parent | $Li^+$ | $Mg^{2+}$ |
|---|---|---|---|
| | NICS (1) | NICS (1) | NICS (1) |
| **1P–σ′$_{1P}$** | -10.27 | -9.64 | -a- |
| **2P–σ′$_{2aP}$** | -9.91 | -9.31 | -a- |
| **3P–σ′$_{1P}$** | -9.38 | -9.10 | -a- |
| **4P–σ′$_{1P}$** | -9.30 | -9.00 | -a- |
| **5P–σ′$_{3aP}$** | -9.24 | -8.97 | -8.59 |
| **6P–σ′$_{2aP}$** | -8.88 | -8.77 | -a- |
| **7P–σ′$_{1P}$** | -8.77 | -8.58 | -a- |
| **8P–σ′$_{3bP}$** | -8.76 | -8.80 | -8.02 |
| **9P–σ′$_{3aP}$** | -8.47 | -8.47 | -7.73 |
| **10P–σ′$_{2aP}$** | -8.31 | -8.52 | -7.16 |
| **11P–σ′$_{3aP}$** | -8.60 | -9.09 | -a- |
| **16P–σ′$_{2aN}$** | -9.30 | -8.63 | -8.59 |
| **17P–σ′$_{1N}$** | -9.73 | -8.71 | -7.40 |
| **18P–σ′$_{3aN}$** | -8.39 | -7.72 | -a- |
| **19P–σ′$_{2aN}$** | -8.91 | -8.18 | -7.83 |
| **20P–σ′$_{1N}$** | -9.26 | -8.76 | -6.77 |
| **21P–σ′$_{2aN}$** | -8.72 | -8.34 | -8.10 |
| **22P–σ′$_{2aN}$** | -8.58 | -8.21 | -8.01 |
| **23P–σ′$_{1N}$** | -8.99 | -8.37 | -3.29 |
| **24P–σ′$_{3bN}$** | -7.62 | -7.43 | -7.23 |
| **25P–σ′$_{2aN}$** | -8.09 | -8.14 | -8.01 |
| **26P–σ′$_{2aN}$** | -8.21 | -7.83 | -7.80 |
| **27P– σ′$_{3aN}$** | -7.73 | -6.99 | -a- |
| **39P– σ′$_{2aN}$** | -7.90 | -8.30 | -8.56 |
| **40P– σ′$_{3bN}$** | -7.06 | -7.13 | -6.71 |
| **41P–σ′$_{3aN}$** | -6.65 | -7.33 | -a- |
| **42P– σ″$_{2N}$** | -7.41 | -8.12 | -7.60 |
| **44P– σ″$_{3N}$** | -6.62 | -7.62 | -7.03 |
| **45P– σ′$_{2aN}$** | -7.03 | -5.97 | -4.94 |
| **46P– σ′$_{2aN}$** | -5.86 | -6.18 | -a- |

[-a-] the corresponding complexes were not localized as minima in potential energy surface.

Table S10: Comparison of the total IE obtained from HF-SAPT, DFT-SAPT (B3LYP and PBE0AC) with CCSD(T)./cc-pVTZ.

| Complex | CCSD(T)/cc-pVTZ | HF/cc-pVDZ | PBE0AC/ cc-pVDZ | B3LYP/cc-pVDZ |
|---|---|---|---|---|
| **Ben-π** | -36.60 | -38.00 | -40.03 | -38.75 |
| **1N–π** | -28.24 | -29.21 | -30.45 | -29.54 |
| **3N–π** | -19.38 | -19.80 | -20.41 | -19.79 |
| **4N–π** | -19.31 | -19.84 | -20.33 | -19.65 |
| **7N–π** | -9.78 | -9.62 | -9.58 | -9.25 |
| **1P–π** | -34.61 | -34.48 | -36.92 | -35.68 |
| **2P–π** | -30.28 | -29.99 | -32.87 | -31.74 |
| **3P–π** | -31.46 | -32.01 | -34.65 | -33.44 |
| **4P–π** | -31.18 | -31.63 | -34.33 | -33.14 |
| **5P–π** | -27.72 | -26.41 | -29.88 | -28.74 |
| **6P–π** | -28.92 | -28.32 | -31.62 | -30.47 |
| **7P–π** | -29.91 | -30.27 | -33.09 | -31.87 |
| **8P–π** | -25.99 | -23.73 | -27.93 | -26.76 |
| **9P–π** | -26.94 | -25.40 | -29.28 | -28.10 |
| **10P–π** | -28.41 | -26.57 | -30.96 | -29.87 |
| **11P–π** | -25.50 | -21.77 | -27.41 | -26.29 |
| **13–π** | -26.54 | -27.23 | -28.62 | -27.72 |
| **14–π** | -26.02 | -26.36 | -27.93 | -27.11 |
| **15–π** | -25.92 | -26.57 | -27.74 | -26.93 |
| **18N–π** | -18.67 | -18.66 | -19.57 | -18.93 |
| **19N–π** | -18.63 | -18.85 | -19.40 | -18.89 |
| **20N–π** | -18.49 | -18.18 | -19.22 | -18.73 |
| **21N–π** | -18.83 | -19.01 | -19.71 | -19.09 |
| **32–π** | -18.48 | -18.30 | -19.40 | -18.81 |
| **33–π** | -18.76 | -18.23 | -19.72 | -19.14 |
| **34–π** | -19.40 | -18.25 | -19.81 | -19.65 |
| **36–π** | -19.04 | -18.51 | -19.74 | -19.19 |
| **37–π** | -19.40 | -19.43 | -20.34 | -19.80 |
| **38–π** | -20.91 | -20.67 | -22.51 | -21.97 |
| **16P–π** | -24.17 | -23.74 | -25.73 | -24.94 |
| **17P–π** | -23.36 | -22.67 | -24.60 | -23.90 |
| **18P–π** | -25.77 | -26.32 | -28.05 | -27.12 |
| **19P–π** | -24.80 | -25.22 | -26.70 | -25.84 |
| **20P–π** | -24.74 | -24.73 | -26.56 | -25.78 |
| **21P–π** | -24.92 | -25.12 | -26.97 | -26.11 |
| **23P–π** | -21.52 | -19.77 | -22.21 | -21.57 |
| **24P–π** | -24.54 | -24.23 | -26.60 | -25.76 |
| **25P–π** | -22.51 | -23.69 | -26.08 | -25.31 |
| **26P–π** | -23.72 | -22.67 | -25.51 | -24.73 |
| **27P–π** | -24.46 | -24.83 | -26.76 | -25.83 |
| **39P–π** | -22.04 | -18.42 | -23.28 | -22.65 |
| **40P–π** | -22.72 | -21.67 | -25.58 | -25.20 |
| **41P–π** | -26.52 | -25.01 | -28.47 | -27.84 |

Table S11: Comparison of the existing experimental results with the BE value obtained at CCSD(T)/cc-pVTZ level.

| Metal complexes | Experimental* kcal/mol | CCSD(T)/cc-pVTZ kcal/mol |
|---|---|---|
| 1N-$Li^+$ | 43.23 | 44.50 |
| 2N-$Li^+$ | 55.99 | 54.06 |
| 3N-$Li^+$ | 36.85 | 38.86 |
| 4N-$Li^+$ | 35.61 | 36.98 |
| 7N-$Li^+$ | 29.72 | 32.72 |

* R. Amunugama and M. T. Rodgers, *Int. J. Mass. Spectrom.*, 2000, **195/196**, 439-457.

Table S12: MP2/cc-pVTZ optimized geometries for the N-analogues parent heteroaromatics.

**Ben**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.393297 | 0.000000 |
| 6 | 1.206630 | 0.696648 | 0.000000 |
| 6 | 1.206630 | -0.696648 | 0.000000 |
| 6 | 0.000000 | -1.393297 | 0.000000 |
| 6 | -1.206630 | -0.696648 | 0.000000 |
| 6 | -1.206630 | 0.696648 | 0.000000 |
| 1 | 0.000000 | 2.474527 | 0.000000 |
| 1 | 2.143003 | 1.237263 | 0.000000 |
| 1 | 2.143003 | -1.237263 | 0.000000 |
| 1 | 0.000000 | -2.474527 | 0.000000 |
| 1 | -2.143003 | -1.237263 | 0.000000 |
| 1 | -2.143003 | 1.237263 | 0.000000 |

**1N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 1.422191 |
| 6 | 0.000000 | 1.141213 | 0.719583 |
| 6 | 0.000000 | 1.193994 | -0.671700 |
| 6 | 0.000000 | 0.000000 | -1.385109 |
| 6 | 0.000000 | -1.193994 | -0.671700 |
| 6 | 0.000000 | -1.141213 | 0.719583 |
| 1 | 0.000000 | 2.054755 | 1.301128 |
| 1 | 0.000000 | 2.148858 | -1.177650 |
| 1 | 0.000000 | 0.000000 | -2.466223 |
| 1 | 0.000000 | -2.148858 | -1.177650 |
| 1 | 0.000000 | -2.054755 | 1.301128 |

**2N**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.319390 | -0.063940 |
| 6 | 0.000000 | 0.691357 | 1.179424 |
| 6 | 0.000000 | -0.691357 | 1.179424 |
| 6 | 0.000000 | -1.319390 | -0.063940 |
| 1 | 0.000000 | 2.397731 | -0.148370 |
| 1 | 0.000000 | 1.268237 | 2.092979 |
| 1 | 0.000000 | -1.268237 | 2.092979 |
| 1 | 0.000000 | -2.397731 | -0.148370 |
| 7 | 0.000000 | 0.669007 | -1.233931 |
| 7 | 0.000000 | -0.669007 | -1.233931 |

**3N**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.183471 | 0.623479 |
| 6 | 0.000000 | 0.000000 | -1.307575 |
| 6 | 0.000000 | -1.183471 | 0.623479 |
| 6 | 0.000000 | 0.000000 | 1.349752 |
| 1 | 0.000000 | 2.146816 | 1.117520 |
| 1 | 0.000000 | 0.000000 | -2.389610 |
| 1 | 0.000000 | -2.146816 | 1.117520 |
| 1 | 0.000000 | 0.000000 | 2.429417 |
| 7 | 0.000000 | -1.198741 | -0.714975 |
| 7 | 0.000000 | 1.198741 | -0.714975 |

**4N**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.130632 | 0.696015 |
| 6 | 0.000000 | -1.130632 | 0.696015 |
| 6 | 0.000000 | -1.130632 | -0.696015 |
| 6 | 0.000000 | 1.130632 | -0.696015 |
| 1 | 0.000000 | 2.061091 | 1.248826 |
| 1 | 0.000000 | -2.061091 | 1.248826 |
| 1 | 0.000000 | -2.061091 | -1.248826 |
| 1 | 0.000000 | 2.061091 | -1.248826 |
| 7 | 0.000000 | 0.000000 | 1.413509 |
| 7 | 0.000000 | 0.000000 | -1.413509 |

**5N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.160329 | 0.731759 |
| 6 | 0.000000 | -1.167488 | -0.607588 |
| 6 | 0.000000 | 0.000000 | -1.349562 |
| 6 | 0.000000 | 1.167488 | -0.607588 |
| 1 | 0.000000 | -2.147139 | -1.065066 |
| 1 | 0.000000 | 0.000000 | -2.429118 |
| 1 | 0.000000 | 2.147139 | -1.065066 |
| 7 | 0.000000 | 0.000000 | 1.386150 |
| 7 | 0.000000 | -1.160329 | 0.731759 |

**6N**

| | | | |
|---|---|---|---|
| 7 | -1.194851 | 0.684590 | 0.000000 |
| 6 | 1.159706 | -0.634020 | 0.000000 |
| 6 | 0.000000 | 1.282884 | 0.000000 |
| 1 | 2.100557 | -1.169195 | 0.000000 |
| 1 | -0.023827 | 2.363722 | 0.000000 |
| 7 | -1.229794 | -0.652264 | 0.000000 |
| 6 | -0.062265 | -1.301383 | 0.000000 |
| 1 | -0.125078 | -2.380683 | 0.000000 |
| 7 | 1.205174 | 0.696427 | 0.000000 |

**7N**

| | | | |
|---|---|---|---|
| 7 | 1.189346 | 0.686669 | 0.000000 |
| 6 | 0.000000 | 1.293075 | 0.000000 |
| 1 | 0.000000 | 2.375016 | 0.000000 |
| 7 | -1.189346 | 0.686669 | 0.000000 |
| 7 | 0.000000 | -1.373338 | 0.000000 |
| 6 | -1.119836 | -0.646538 | 0.000000 |
| 1 | -2.056824 | -1.187508 | 0.000000 |
| 6 | 1.119836 | -0.646538 | 0.000000 |
| 1 | 2.056824 | -1.187508 | 0.000000 |

**8N**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 0.692873 | 1.100355 |
| 6 | 0.000000 | -0.692873 | 1.100355 |
| 1 | 0.000000 | 1.281169 | 2.007524 |
| 1 | 0.000000 | -1.281169 | 2.007524 |
| 7 | 0.000000 | 1.368324 | -0.047077 |
| 7 | 0.000000 | 0.663607 | -1.182873 |
| 7 | 0.000000 | -0.663607 | -1.182873 |
| 7 | 0.000000 | -1.368324 | -0.047077 |

**9N**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.106730 | 0.631883 |
| 1 | 0.000000 | 2.060853 | 1.140292 |
| 1 | 0.000000 | -2.060853 | 1.140292 |
| 7 | 0.000000 | -1.149832 | -0.705080 |
| 7 | 0.000000 | 0.000000 | -1.370461 |
| 7 | 0.000000 | 1.149832 | -0.705080 |
| 7 | 0.000000 | 0.000000 | 1.371595 |
| 6 | 0.000000 | -1.106730 | 0.631883 |

**10N**

| | | | |
|---|---|---|---|
| 1 | 0.000000 | 0.000000 | 2.341146 |
| 1 | 0.000000 | 0.000000 | -2.341146 |

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.198562 | -0.665447 |
| 7 | 0.000000 | 1.198562 | 0.665447 |
| 7 | 0.000000 | -1.198562 | -0.665447 |
| 6 | 0.000000 | 0.000000 | -1.260825 |
| 7 | 0.000000 | -1.198562 | 0.665447 |
| 6 | 0.000000 | 0.000000 | 1.260825 |

**11N**

| | | | |
|---|---|---|---|
| 1 | 0.000000 | 0.000000 | -2.335920 |
| 7 | 0.000000 | 1.163346 | 0.683557 |
| 7 | 0.000000 | 1.183693 | -0.643204 |
| 7 | 0.000000 | -1.163346 | 0.683557 |
| 7 | 0.000000 | -1.183693 | -0.643204 |
| 6 | 0.000000 | 0.000000 | -1.255321 |
| 7 | 0.000000 | 0.000000 | 1.328986 |

**13**

| | | | |
|---|---|---|---|
| 7 | -0.745546 | -1.181667 | 0.000000 |
| 15 | -1.391865 | 0.341930 | 0.000000 |
| 6 | 0.000000 | 1.388588 | 0.000000 |
| 6 | 1.302486 | 0.899164 | 0.000000 |
| 6 | 1.577601 | -0.466779 | 0.000000 |
| 6 | 0.564008 | -1.426715 | 0.000000 |
| 1 | -0.157653 | 2.461430 | 0.000000 |
| 1 | 2.133938 | 1.594411 | 0.000000 |
| 1 | 2.605426 | -0.803244 | 0.000000 |
| 1 | 0.850517 | -2.475421 | 0.000000 |

**14**

| | | | |
|---|---|---|---|
| 7 | 1.288457 | 0.981815 | 0.000000 |
| 6 | 0.000000 | 1.342100 | 0.000000 |
| 15 | -1.430757 | 0.342181 | 0.000000 |
| 6 | -0.656349 | -1.211523 | 0.000000 |
| 6 | 0.721620 | -1.385581 | 0.000000 |
| 6 | 1.614977 | -0.315165 | 0.000000 |
| 1 | -0.163162 | 2.416299 | 0.000000 |
| 1 | -1.288271 | -2.091967 | 0.000000 |
| 1 | 1.133342 | -2.387520 | 0.000000 |
| 1 | 2.678754 | -0.521212 | 0.000000 |

**15**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | -1.715891 |
| 6 | 0.000000 | 1.154860 | -1.038468 |
| 6 | 0.000000 | 1.311403 | 0.343662 |
| 15 | 0.000000 | 0.000000 | 1.480349 |
| 6 | 0.000000 | -1.311403 | 0.343662 |
| 6 | 0.000000 | -1.154860 | -1.038468 |
| 1 | 0.000000 | 2.042545 | -1.662640 |
| 1 | 0.000000 | 2.321682 | 0.734473 |
| 1 | 0.000000 | -2.321682 | 0.734473 |
| 1 | 0.000000 | -2.042545 | -1.662640 |

**16N**

| | | | |
|---|---|---|---|
| 7 | 1.268736 | 0.972552 | 0.000000 |
| 7 | 0.000000 | 1.380485 | 0.000000 |
| 15 | -1.354833 | 0.412860 | 0.000000 |
| 6 | -0.706559 | -1.206071 | 0.000000 |
| 6 | 0.662961 | -1.404050 | 0.000000 |
| 6 | 1.562597 | -0.333092 | 0.000000 |
| 1 | -1.370922 | -2.062643 | 0.000000 |
| 1 | 1.072360 | -2.407105 | 0.000000 |
| 1 | 2.625910 | -0.535133 | 0.000000 |

**17N**

| | | | |
|---|---|---|---|
| 7 | 1.673762 | -0.318545 | 0.000000 |
| 7 | 1.291546 | 0.960057 | 0.000000 |
| 6 | 0.000000 | 1.309547 | 0.000000 |
| 15 | -1.438264 | 0.316898 | 0.000000 |
| 6 | -0.616458 | -1.203435 | 0.000000 |
| 6 | 0.770465 | -1.309236 | 0.000000 |
| 1 | -0.138378 | 2.385743 | 0.000000 |
| 1 | -1.195649 | -2.118701 | 0.000000 |
| 1 | 1.226788 | -2.292354 | 0.000000 |

**18N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.338164 | 0.407024 |
| 15 | 0.000000 | 0.000000 | 1.378178 |
| 7 | 0.000000 | -1.338164 | 0.407024 |
| 6 | 0.000000 | -1.214531 | -0.921236 |
| 6 | 0.000000 | 0.000000 | -1.606475 |
| 6 | 0.000000 | 1.214531 | -0.921236 |
| 1 | 0.000000 | -2.137504 | -1.495120 |
| 1 | 0.000000 | 0.000000 | -2.687086 |
| 1 | 0.000000 | 2.137504 | -1.495120 |

**19N**

| | | | |
|---|---|---|---|
| 7 | 1.606150 | -0.457470 | 0.000000 |
| 6 | 0.619008 | -1.363869 | 0.000000 |
| 7 | -0.696867 | -1.180465 | 0.000000 |
| 15 | -1.385601 | 0.322835 | 0.000000 |
| 6 | 0.000000 | 1.365525 | 0.000000 |
| 6 | 1.289212 | 0.841814 | 0.000000 |
| 1 | 0.956392 | -2.395568 | 0.000000 |
| 1 | -0.126090 | 2.441439 | 0.000000 |
| 1 | 2.139412 | 1.516323 | 0.000000 |

**20N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.206812 | -1.034681 |
| 6 | 0.000000 | 0.000000 | -1.607311 |
| 7 | 0.000000 | -1.206812 | -1.034681 |
| 6 | 0.000000 | -1.298661 | 0.298228 |
| 15 | 0.000000 | 0.000000 | 1.458748 |
| 6 | 0.000000 | 1.298661 | 0.298228 |
| 1 | 0.000000 | 0.000000 | -2.689734 |
| 1 | 0.000000 | -2.315676 | 0.679588 |
| 1 | 0.000000 | 2.315676 | 0.679588 |

**21N**

| | | | |
|---|---|---|---|
| 7 | -0.689775 | -1.211639 | 0.000000 |
| 15 | -1.391109 | 0.289730 | 0.000000 |
| 6 | 0.000000 | 1.347847 | 0.000000 |
| 7 | 1.286419 | 0.973626 | 0.000000 |
| 6 | 1.572080 | -0.333820 | 0.000000 |
| 6 | 0.632513 | -1.368328 | 0.000000 |
| 1 | -0.163441 | 2.422644 | 0.000000 |
| 1 | 2.625706 | -0.585678 | 0.000000 |
| 1 | 1.000310 | -2.391026 | 0.000000 |

**22N**

| | | | |
|---|---|---|---|
| 7 | 1.619902 | -0.327376 | 0.000000 |
| 7 | 1.264577 | 0.955766 | 0.000000 |
| 7 | 0.000000 | 1.345811 | 0.000000 |
| 15 | -1.363008 | 0.382503 | 0.000000 |
| 6 | -0.661441 | -1.201116 | 0.000000 |

| | | | |
|---|---|---|---|
| 6 | 0.719176 | -1.324435 | 0.000000 |
| 1 | -1.270354 | -2.097108 | 0.000000 |
| 1 | 1.177715 | -2.306545 | 0.000000 |

**23N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.168134 | -1.052289 |
| 7 | 0.000000 | 0.000000 | -1.692038 |
| 7 | 0.000000 | -1.168134 | -1.052289 |
| 6 | 0.000000 | -1.273087 | 0.281395 |
| 15 | 0.000000 | 0.000000 | 1.463549 |
| 6 | 0.000000 | 1.273087 | 0.281395 |
| 1 | 0.000000 | -2.302663 | 0.623171 |
| 1 | 0.000000 | 2.302663 | 0.623171 |

**24N**

| | | | |
|---|---|---|---|
| 7 | -1.264240 | -0.966359 | 0.000000 |
| 7 | -1.326854 | 0.368240 | 0.000000 |
| 15 | 0.000000 | 1.365684 | 0.000000 |
| 7 | 1.352683 | 0.395531 | 0.000000 |
| 6 | 1.182512 | -0.919916 | 0.000000 |
| 6 | -0.065970 | -1.560956 | 0.000000 |
| 1 | 2.076175 | -1.539482 | 0.000000 |
| 1 | -0.106549 | -2.642434 | 0.000000 |

**25N**

| | | | |
|---|---|---|---|
| 7 | -0.640070 | -1.213818 | 0.000000 |
| 7 | 0.677629 | -1.413567 | 0.000000 |
| 6 | 1.519820 | -0.374347 | 0.000000 |
| 7 | 1.267867 | 0.943290 | 0.000000 |
| 6 | 0.000000 | 1.352363 | 0.000000 |
| 15 | -1.378809 | 0.276335 | 0.000000 |
| 1 | 2.564618 | -0.654906 | 0.000000 |
| 1 | -0.139383 | 2.430444 | 0.000000 |

**26N**

| | | | |
|---|---|---|---|
| 7 | 1.286242 | 0.948845 | 0.000000 |
| 7 | 1.622589 | -0.342804 | 0.000000 |
| 6 | 0.681446 | -1.301116 | 0.000000 |
| 7 | -0.645845 | -1.206774 | 0.000000 |
| 15 | -1.392902 | 0.266520 | 0.000000 |
| 6 | 0.000000 | 1.319907 | 0.000000 |
| 1 | 1.098024 | -2.302611 | 0.000000 |
| 1 | -0.134077 | 2.397194 | 0.000000 |

**27N**

| | | | |
|---|---|---|---|
| 6 | -0.939563 | 1.147983 | -0.000001 |
| 6 | -0.939563 | -1.147983 | -0.000001 |
| 1 | -1.549694 | 2.046209 | 0.000002 |
| 1 | -1.549694 | -2.046209 | 0.000002 |
| 7 | -1.627823 | 0.000000 | 0.000000 |
| 7 | 0.380451 | -1.322681 | 0.000000 |
| 7 | 0.380451 | 1.322681 | 0.000000 |
| 15 | 1.362840 | 0.000000 | 0.000000 |

**28**

| | | | |
|---|---|---|---|
| 7 | 1.744972 | -0.619692 | 0.000000 |
| 7 | 1.467201 | 0.676143 | 0.000000 |
| 15 | 0.000000 | 1.466279 | 0.000000 |
| 15 | -1.571253 | 0.024341 | 0.000000 |
| 6 | -0.606645 | -1.420689 | 0.000000 |
| 6 | 0.781236 | -1.552865 | 0.000000 |
| 1 | -1.155680 | -2.357094 | 0.000000 |
| 1 | 1.191718 | -2.556046 | 0.000000 |

**29**

| | | | |
|---|---|---|---|
| 7 | -0.056929 | -1.729910 | 0.000000 |
| 7 | -1.225389 | -1.094263 | 0.000000 |
| 15 | -1.533119 | 0.541861 | 0.000000 |
| 6 | 0.000000 | 1.364109 | 0.000000 |
| 15 | 1.557387 | 0.617278 | 0.000000 |
| 6 | 1.113258 | -1.080596 | 0.000000 |
| 1 | -0.019821 | 2.450775 | 0.000000 |
| 1 | 1.952476 | -1.769733 | 0.000000 |

**30**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.663683 | -1.371195 |
| 15 | 0.000000 | -1.696841 | -0.064333 |
| 6 | 0.000000 | -0.691706 | 1.372695 |
| 6 | 0.000000 | 0.691706 | 1.372695 |
| 1 | 0.000000 | -1.211500 | 2.327189 |
| 1 | 0.000000 | 1.211500 | 2.327189 |
| 15 | 0.000000 | 1.696841 | -0.064333 |
| 7 | 0.000000 | -0.663683 | -1.371195 |

**31**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.667188 | 1.725918 |
| 7 | 0.000000 | -0.667188 | 1.725918 |
| 6 | 0.000000 | -1.403675 | 0.610728 |
| 15 | 0.000000 | -1.050645 | -1.106052 |
| 15 | 0.000000 | 1.050645 | -1.106052 |
| 6 | 0.000000 | 1.403675 | 0.610728 |
| 1 | 0.000000 | -2.465338 | 0.844990 |
| 1 | 0.000000 | 2.465338 | 0.844990 |

**32**

| | | | |
|---|---|---|---|
| 7 | -1.264914 | -1.038916 | 0.000000 |
| 15 | -1.457039 | 0.600084 | 0.000000 |
| 7 | 0.000000 | 1.351892 | 0.000000 |
| 15 | 1.485176 | 0.645031 | 0.000000 |
| 6 | 1.176056 | -1.068048 | 0.000000 |
| 6 | -0.087579 | -1.663491 | 0.000000 |
| 1 | 2.037529 | -1.726734 | 0.000000 |
| 1 | -0.136044 | -2.751587 | 0.000000 |

**33**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.351128 | -0.724662 |
| 15 | 0.000000 | 0.000000 | -1.675940 |
| 7 | 0.000000 | -1.351128 | -0.724662 |
| 6 | 0.000000 | -1.347405 | 0.604485 |
| 15 | 0.000000 | 0.000000 | 1.725721 |
| 6 | 0.000000 | 1.347405 | 0.604485 |
| 1 | 0.000000 | -2.332831 | 1.072368 |
| 1 | 0.000000 | 2.332831 | 1.072368 |

**34**

| | | | |
|---|---|---|---|
| 7 | 0.739338 | -1.647319 | 0.000000 |
| 6 | 1.627047 | -0.639015 | 0.000000 |
| 7 | 1.443665 | 0.669315 | 0.000000 |
| 15 | 0.000000 | 1.481076 | 0.000000 |
| 15 | -1.540562 | 0.027977 | 0.000000 |
| 6 | -0.573986 | -1.437868 | 0.000000 |
| 1 | 2.661521 | -0.968826 | 0.000000 |

| | | | |
|---|---|---|---|
| 1 | -1.152486 | -2.359646 | 0.000000 |

**35**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.208592 | 1.060506 |
| 6 | 0.000000 | 0.000000 | 1.618009 |
| 7 | 0.000000 | -1.208592 | 1.060506 |
| 15 | 0.000000 | -1.537028 | -0.555426 |
| 6 | 0.000000 | 0.000000 | -1.358856 |
| 15 | 0.000000 | 1.537028 | -0.555426 |
| 1 | 0.000000 | 0.000000 | 2.706341 |
| 1 | 0.000000 | 0.000000 | -2.445548 |

**36**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.515283 | 0.540657 |
| 6 | 0.000000 | 0.702099 | 1.590340 |
| 6 | 0.000000 | -0.702099 | 1.590340 |
| 7 | 0.000000 | -1.515283 | 0.540657 |
| 15 | 0.000000 | -1.071891 | -1.059340 |
| 15 | 0.000000 | 1.071891 | -1.059340 |
| 1 | 0.000000 | 1.188588 | 2.563463 |
| 1 | 0.000000 | -1.188588 | 2.563463 |

**37**

| | | | |
|---|---|---|---|
| 7 | 0.000145 | 1.744123 | 0.000000 |
| 6 | -0.000068 | 1.084457 | 1.166394 |
| 15 | -0.000068 | -0.641586 | 1.483416 |
| 7 | 0.000306 | -1.348573 | 0.000000 |
| 15 | -0.000068 | -0.641586 | -1.483416 |
| 6 | -0.000068 | 1.084457 | -1.166394 |
| 1 | -0.000151 | 1.732615 | 2.041248 |
| 1 | -0.000151 | 1.732615 | -2.041248 |

**38**

| | | | |
|---|---|---|---|
| 6 | -0.599359 | 1.351743 | 0.000030 |
| 6 | 0.599374 | -1.351720 | 0.000030 |
| 1 | -1.066007 | 2.339356 | 0.000071 |
| 1 | 1.066028 | -2.339330 | 0.000070 |
| 15 | -1.705349 | -0.016238 | -0.000011 |
| 15 | 1.705338 | 0.016232 | -0.000011 |
| 7 | -0.731245 | -1.355725 | -0.000011 |
| 7 | 0.731253 | 1.355716 | -0.000011 |

**39N**

| | | | |
|---|---|---|---|
| 7 | 0.482387 | -1.830524 | 0.000000 |
| 15 | -1.143473 | -1.563572 | 0.000000 |
| 15 | -1.694801 | 0.501871 | 0.000000 |
| 15 | 0.000000 | 1.757261 | 0.000000 |
| 15 | 1.826801 | 0.685228 | 0.000000 |
| 6 | 1.550100 | -1.049898 | 0.000000 |
| 1 | 2.494787 | -1.598772 | 0.000000 |

**40N**

| | | | |
|---|---|---|---|
| 7 | -1.663320 | -0.474481 | 0.000000 |
| 15 | -1.651901 | 1.161019 | 0.000000 |
| 6 | 0.000000 | 1.721486 | 0.000000 |
| 15 | 1.589203 | 1.007705 | 0.000000 |
| 15 | 1.441401 | -1.102205 | 0.000000 |
| 15 | -0.606005 | -1.721094 | 0.000000 |
| 1 | 0.052764 | 2.811084 | 0.000000 |

**41N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 1.648731 |
| 15 | 0.000000 | 1.541237 | 1.093351 |
| 15 | 0.000000 | 1.626123 | -1.051116 |
| 6 | 0.000000 | 0.000000 | -1.673938 |
| 15 | 0.000000 | -1.626123 | -1.051116 |
| 15 | 0.000000 | -1.541237 | 1.093351 |
| 1 | 0.000000 | 0.000000 | -2.764535 |

**42N**

| | | | |
|---|---|---|---|
| 15 | -1.553852 | 0.023316 | 0.000000 |
| 15 | 0.000000 | 1.465737 | 0.000000 |
| 7 | 1.442220 | 0.623883 | 0.000000 |
| 7 | 1.719464 | -0.662935 | 0.000000 |
| 7 | 0.783741 | -1.615260 | 0.000000 |
| 6 | -0.538627 | -1.401743 | 0.000000 |
| 1 | -1.078436 | -2.345150 | 0.000000 |

**43N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.162013 | 1.084910 |
| 7 | 0.000000 | 0.000000 | 1.716182 |
| 7 | 0.000000 | -1.162013 | 1.084910 |
| 15 | 0.000000 | -1.520267 | -0.548321 |
| 6 | 0.000000 | 0.000000 | -1.380787 |
| 15 | 0.000000 | 1.520267 | -0.548321 |
| 1 | 0.000000 | 0.000000 | -2.467664 |

**44N**

| | | | |
|---|---|---|---|
| 7 | -0.631736 | -1.430513 | 0.000000 |
| 15 | -1.513753 | -0.028628 | 0.000000 |
| 15 | 0.000000 | 1.484612 | 0.000000 |
| 7 | 1.450733 | 0.658788 | 0.000000 |
| 7 | 1.681335 | -0.646141 | 0.000000 |
| 6 | 0.689208 | -1.556856 | 0.000000 |
| 1 | 1.068730 | -2.573564 | 0.000000 |

**45N**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.371249 | 0.000000 |
| 15 | -1.447073 | 0.576438 | 0.000000 |
| 7 | -1.216457 | -1.070002 | 0.000000 |
| 7 | -0.062451 | -1.737276 | 0.000000 |
| 6 | 1.106647 | -1.080846 | 0.000000 |
| 15 | 1.470675 | 0.643129 | 0.000000 |
| 1 | 1.958434 | -1.756221 | 0.000000 |

**46N**

| | | | |
|---|---|---|---|
| 7 | -0.058225 | -1.512374 | 0.000000 |
| 7 | 1.164791 | -0.987471 | 0.000000 |
| 15 | 1.547230 | 0.634973 | 0.000000 |
| 6 | 0.000000 | 1.489266 | 0.000000 |
| 7 | -1.215092 | 0.959563 | 0.000000 |
| 15 | -1.499401 | -0.683951 | 0.000000 |
| 1 | 0.042250 | 2.581048 | 0.000000 |

**47N**

| | | | |
|---|---|---|---|
| 6 | -0.000012 | 1.617790 | 0.000026 |
| 1 | -0.000035 | 2.706739 | 0.000724 |
| 7 | 1.204990 | 1.046150 | -0.000052 |
| 7 | 0.000031 | -1.366356 | 0.000296 |
| 7 | -1.205006 | 1.046103 | -0.000044 |

| | | | |
|---|---|---|---|
| 15 | 1.443936 | -0.583153 | -0.000074 |
| 15 | -1.443936 | -0.583164 | -0.000077 |

Table S13: MP2/cc-pVTZ optimized geometries for the P-analogues parent heteroaromatics

**1P**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 0.000000 | 1.486931 |
| 6 | 0.000000 | 1.331554 | 0.368734 |
| 6 | 0.000000 | 1.222631 | -1.018110 |
| 6 | 0.000000 | 0.000000 | -1.686950 |
| 6 | 0.000000 | -1.222631 | -1.018110 |
| 6 | 0.000000 | -1.331554 | 0.368734 |
| 1 | 0.000000 | 2.325922 | 0.800329 |
| 1 | 0.000000 | 2.129640 | -1.610842 |
| 1 | 0.000000 | 0.000000 | -2.768724 |
| 1 | 0.000000 | -2.129640 | -1.610842 |
| 1 | 0.000000 | -2.325922 | 0.800329 |

**2P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.506665 | 0.558947 |
| 6 | 0.000000 | 0.698273 | 1.688236 |
| 6 | 0.000000 | -0.698273 | 1.688236 |
| 6 | 0.000000 | -1.506665 | 0.558947 |
| 1 | 0.000000 | 2.578792 | 0.732333 |
| 1 | 0.000000 | 1.189386 | 2.654403 |
| 1 | 0.000000 | -1.189386 | 2.654403 |
| 1 | 0.000000 | -2.578792 | 0.732333 |
| 15 | 0.000000 | -1.055300 | -1.124656 |
| 15 | 0.000000 | 1.055300 | -1.124656 |

**3P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.239687 | 1.074478 |
| 6 | 0.000000 | 0.000000 | -1.340068 |
| 6 | 0.000000 | -1.239687 | 1.074478 |
| 6 | 0.000000 | 0.000000 | 1.708356 |
| 1 | 0.000000 | 2.115713 | 1.714091 |
| 1 | 0.000000 | 0.000000 | -2.427256 |
| 1 | 0.000000 | -2.115713 | 1.714091 |
| 1 | 0.000000 | 0.000000 | 2.793873 |
| 15 | 0.000000 | -1.582176 | -0.629942 |
| 15 | 0.000000 | 1.582176 | -0.629942 |

**4P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.355763 | 0.694212 |
| 6 | 0.000000 | -1.355763 | 0.694212 |
| 6 | 0.000000 | -1.355763 | -0.694212 |
| 6 | 0.000000 | 1.355763 | -0.694212 |
| 1 | 0.000000 | 2.324480 | 1.186195 |
| 1 | 0.000000 | -2.324480 | 1.186195 |
| 1 | 0.000000 | -2.324480 | -1.186195 |
| 1 | 0.000000 | 2.324480 | -1.186195 |
| 15 | 0.000000 | 0.000000 | -1.786959 |
| 15 | 0.000000 | 0.000000 | 1.786959 |

**5P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.251857 | -1.312140 |
| 6 | 0.000000 | 0.000000 | -1.922520 |
| 6 | 0.000000 | -1.251857 | -1.312140 |
| 1 | 0.000000 | 2.100878 | -1.990611 |
| 1 | 0.000000 | 0.000000 | -3.008100 |
| 1 | 0.000000 | -2.100878 | -1.990611 |
| 15 | 0.000000 | -1.733449 | 0.360415 |
| 15 | 0.000000 | 0.000000 | 1.563846 |
| 15 | 0.000000 | 1.733449 | 0.360415 |

**6P**

| | | | |
|---|---|---|---|
| 6 | 1.603307 | -0.715781 | 0.000000 |
| 6 | 0.000000 | 1.528103 | 0.000000 |
| 1 | 2.592905 | -1.165357 | 0.000000 |
| 1 | -0.101041 | 2.612969 | 0.000000 |
| 6 | 0.536261 | -1.602769 | 0.000000 |
| 1 | 0.801095 | -2.658193 | 0.000000 |
| 15 | 1.659492 | 1.026880 | 0.000000 |
| 15 | -1.542990 | 0.726520 | 0.000000 |
| 15 | -1.191860 | -1.356516 | 0.000000 |

**7P**

| | | | |
|---|---|---|---|
| 6 | -0.795738 | 1.378259 | 0.000000 |
| 1 | -1.339747 | 2.320509 | 0.000000 |
| 6 | -0.795738 | -1.378259 | 0.000000 |
| 1 | -1.339747 | -2.320509 | 0.000000 |
| 6 | 1.591477 | 0.000000 | 0.000000 |
| 1 | 2.679493 | 0.000000 | 0.000000 |
| 15 | 0.925053 | 1.602239 | 0.000000 |
| 15 | 0.925053 | -1.602239 | 0.000000 |
| 15 | -1.850106 | 0.000000 | 0.000000 |

**8P**

| | | | |
|---|---|---|---|
| 6 | 0.503347 | -1.824406 | 0.000000 |
| 6 | 1.613543 | -0.989103 | 0.000000 |
| 1 | 0.735348 | -2.887846 | 0.000000 |
| 1 | 2.571073 | -1.506659 | 0.000000 |
| 15 | -1.223285 | -1.570867 | 0.000000 |
| 15 | -1.688505 | 0.490398 | 0.000000 |
| 15 | -0.003387 | 1.758271 | 0.000000 |
| 15 | 1.848296 | 0.740185 | 0.000000 |

**9P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.397329 | 1.043229 |
| 1 | 0.000000 | 2.312820 | 1.635450 |
| 15 | 0.000000 | -1.766375 | -0.656132 |
| 15 | 0.000000 | 0.000000 | -1.814822 |
| 15 | 0.000000 | 1.766375 | -0.656132 |
| 6 | 0.000000 | -1.397329 | 1.043229 |
| 15 | 0.000000 | 0.000000 | 2.074444 |
| 1 | 0.000000 | -2.312820 | 1.635450 |

**10P**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 1.629639 | 1.058606 |
| 15 | 0.000000 | 1.629639 | -1.058606 |
| 6 | 0.000000 | 0.000000 | 1.665307 |
| 15 | 0.000000 | -1.629639 | 1.058606 |
| 1 | 0.000000 | 0.000000 | 2.756669 |
| 15 | 0.000000 | -1.629639 | -1.058606 |
| 6 | 0.000000 | 0.000000 | -1.665307 |
| 1 | 0.000000 | 0.000000 | -2.756669 |

**11P**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 1.647433 | -1.298111 |
| 15 | 0.000000 | 1.805911 | 0.813166 |
| 6 | 0.000000 | 0.000000 | -1.863745 |
| 15 | 0.000000 | -1.647433 | -1.298111 |
| 1 | 0.000000 | 0.000000 | -2.955741 |
| 15 | 0.000000 | -1.805911 | 0.813166 |

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 0.000000 | 1.912436 |

**16P**

| | | | |
|---|---|---|---|
| 7 | 1.460596 | 0.711066 | 0.000000 |
| 15 | 0.000000 | 1.490973 | 0.000000 |
| 15 | -1.556708 | 0.038750 | 0.000000 |
| 6 | -0.650578 | -1.451286 | 0.000000 |
| 6 | 0.727593 | -1.624030 | 0.000000 |
| 6 | 1.679072 | -0.597205 | 0.000000 |
| 1 | -1.248455 | -2.357680 | 0.000000 |
| 1 | 1.112888 | -2.636924 | 0.000000 |
| 1 | 2.725494 | -0.893576 | 0.000000 |

**17P**

| | | | |
|---|---|---|---|
| 7 | 1.698737 | -0.746364 | 0.000000 |
| 6 | 1.466310 | 0.566216 | 0.000000 |
| 15 | 0.000000 | 1.522745 | 0.000000 |
| 15 | -1.537850 | 0.082386 | 0.000000 |
| 6 | -0.665628 | -1.424711 | 0.000000 |
| 6 | 0.705461 | -1.645657 | 0.000000 |
| 1 | 2.376541 | 1.163161 | 0.000000 |
| 1 | -1.285733 | -2.315637 | 0.000000 |
| 1 | 1.048929 | -2.675047 | 0.000000 |

**18P**

| | | | |
|---|---|---|---|
| 7 | 1.698737 | -0.746364 | 0.000000 |
| 6 | 1.466310 | 0.566216 | 0.000000 |
| 15 | 0.000000 | 1.522745 | 0.000000 |
| 15 | -1.537850 | 0.082386 | 0.000000 |
| 6 | -0.665628 | -1.424711 | 0.000000 |
| 6 | 0.705461 | -1.645657 | 0.000000 |
| 1 | 2.376541 | 1.163161 | 0.000000 |
| 1 | -1.285733 | -2.315637 | 0.000000 |
| 1 | 1.048929 | -2.675047 | 0.000000 |

**19P**

| | | | |
|---|---|---|---|
| 7 | -1.268325 | -1.061895 | 0.000000 |
| 15 | -1.551101 | 0.564224 | 0.000000 |
| 6 | 0.000000 | 1.346448 | 0.000000 |
| 15 | 1.575374 | 0.623075 | 0.000000 |
| 6 | 1.183259 | -1.070230 | 0.000000 |
| 6 | -0.079804 | -1.661662 | 0.000000 |
| 1 | -0.019648 | 2.433477 | 0.000000 |
| 1 | 2.030009 | -1.747347 | 0.000000 |
| 1 | -0.116912 | -2.749680 | 0.000000 |

**20P**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 1.736538 |
| 6 | 0.000000 | 1.171390 | 1.092015 |
| 15 | 0.000000 | 1.567229 | -0.608997 |
| 6 | 0.000000 | 0.000000 | -1.345066 |
| 15 | 0.000000 | -1.567229 | -0.608997 |
| 6 | 0.000000 | -1.171390 | 1.092015 |
| 1 | 0.000000 | 2.032285 | 1.756107 |
| 1 | 0.000000 | 0.000000 | -2.431842 |
| 1 | 0.000000 | -2.032285 | 1.756107 |

**21P**

| | | | |
|---|---|---|---|
| 7 | -1.216020 | 0.940645 | 0.000000 |
| 15 | -1.598415 | -0.668403 | 0.000000 |
| 6 | -0.074811 | -1.521327 | 0.000000 |
| 6 | 1.192316 | -0.954263 | 0.000000 |
| 15 | 1.591005 | 0.740570 | 0.000000 |
| 6 | 0.000000 | 1.475510 | 0.000000 |
| 1 | -0.144523 | -2.606160 | 0.000000 |
| 1 | 2.045586 | -1.626615 | 0.000000 |
| 1 | 0.017202 | 2.566219 | 0.000000 |

**22P**

| | | | |
|---|---|---|---|
| 7 | -1.271718 | -1.307058 | 0.000000 |
| 15 | -1.692541 | 0.284767 | 0.000000 |
| 15 | 0.000000 | 1.581461 | 0.000000 |
| 15 | 1.714906 | 0.355259 | 0.000000 |
| 6 | 1.188348 | -1.306661 | 0.000000 |
| 6 | -0.078019 | -1.890337 | 0.000000 |
| 1 | 2.014277 | -2.012285 | 0.000000 |
| 1 | -0.109698 | -2.978618 | 0.000000 |

**23P**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | -1.950027 |
| 6 | 0.000000 | 1.182516 | -1.331231 |
| 15 | 0.000000 | 1.707850 | 0.336176 |
| 15 | 0.000000 | 0.000000 | 1.572987 |
| 15 | 0.000000 | -1.707850 | 0.336176 |
| 6 | 0.000000 | -1.182516 | -1.331231 |
| 1 | 0.000000 | 2.019798 | -2.027552 |
| 1 | 0.000000 | -2.019798 | -2.027552 |

**24P**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.526332 | 0.000000 |
| 15 | -1.454432 | 0.763651 | 0.000000 |
| 15 | -1.191246 | -1.357109 | 0.000000 |
| 6 | 0.539280 | -1.606589 | 0.000000 |
| 6 | 1.589844 | -0.697669 | 0.000000 |
| 15 | 1.566557 | 1.054620 | 0.000000 |
| 1 | 0.818866 | -2.658021 | 0.000000 |
| 1 | 2.593216 | -1.118181 | 0.000000 |

**25P**

| | | | |
|---|---|---|---|
| 7 | 0.516456 | -1.619292 | 0.000000 |
| 15 | -1.115326 | -1.352972 | 0.000000 |
| 15 | -1.549339 | 0.739303 | 0.000000 |
| 6 | 0.000000 | 1.526814 | 0.000000 |
| 15 | 1.646019 | 0.977675 | 0.000000 |
| 6 | 1.536680 | -0.773959 | 0.000000 |
| 1 | -0.071665 | 2.613599 | 0.000000 |
| 1 | 2.516077 | -1.255777 | 0.000000 |

**26P**

| | | | |
|---|---|---|---|
| 7 | 1.620669 | -0.698253 | 0.000000 |
| 15 | 1.640775 | 0.953905 | 0.000000 |
| 6 | 0.000000 | 1.524724 | 0.000000 |
| 15 | -1.545254 | 0.726382 | 0.000000 |
| 15 | -1.146813 | -1.348956 | 0.000000 |
| 6 | 0.600927 | -1.541462 | 0.000000 |
| 1 | -0.075110 | 2.611932 | 0.000000 |
| 1 | 0.894249 | -2.593702 | 0.000000 |

**27P**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | -1.587075 |
| 15 | 0.000000 | 1.509448 | -0.953481 |
| 6 | 0.000000 | 1.370558 | 0.782038 |
| 15 | 0.000000 | 0.000000 | 1.848732 |

| | | | |
|---|---|---|---|
| 6 | 0.000000 | -1.370558 | 0.782038 |
| 15 | 0.000000 | -1.509448 | -0.953481 |
| 1 | 0.000000 | 2.328225 | 1.299260 |
| 1 | 0.000000 | -2.328225 | 1.299260 |

**39P**

| | | | |
|---|---|---|---|
| 7 | 0.482387 | -1.830524 | 0.000000 |
| 15 | -1.143473 | -1.563572 | 0.000000 |
| 15 | -1.694801 | 0.501871 | 0.000000 |
| 15 | 0.000000 | 1.757261 | 0.000000 |
| 15 | 1.826801 | 0.685228 | 0.000000 |
| 6 | 1.550100 | -1.049898 | 0.000000 |
| 1 | 2.494787 | -1.598772 | 0.000000 |

**40P**

| | | | |
|---|---|---|---|
| 7 | -1.663320 | -0.474481 | 0.000000 |
| 15 | -1.651901 | 1.161019 | 0.000000 |
| 6 | 0.000000 | 1.721486 | 0.000000 |
| 15 | 1.589203 | 1.007705 | 0.000000 |
| 15 | 1.441401 | -1.102205 | 0.000000 |
| 15 | -0.606005 | -1.721094 | 0.000000 |
| 1 | 0.052764 | 2.811084 | 0.000000 |

**41P**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 1.648731 |
| 15 | 0.000000 | 1.541237 | 1.093351 |
| 15 | 0.000000 | 1.626123 | -1.051116 |
| 6 | 0.000000 | 0.000000 | -1.673938 |
| 15 | 0.000000 | -1.626123 | -1.051116 |
| 15 | 0.000000 | -1.541237 | 1.093351 |
| 1 | 0.000000 | 0.000000 | -2.764535 |

**42P**

| | | | |
|---|---|---|---|
| 7 | -0.058399 | -1.967360 | 0.000000 |
| 7 | -1.227833 | -1.346134 | 0.000000 |
| 15 | -1.656533 | 0.261243 | 0.000000 |
| 15 | 0.000000 | 1.610254 | 0.000000 |
| 15 | 1.681108 | 0.340523 | 0.000000 |
| 6 | 1.115826 | -1.325149 | 0.000000 |
| 1 | 1.940042 | -2.034964 | 0.000000 |

**44P**

| | | | |
|---|---|---|---|
| 7 | 0.567143 | -1.604482 | 0.000000 |
| 7 | 1.593482 | -0.773117 | 0.000000 |
| 15 | 1.629874 | 0.892937 | 0.000000 |
| 6 | 0.000000 | 1.525329 | 0.000000 |
| 15 | -1.559430 | 0.763433 | 0.000000 |
| 15 | -1.076413 | -1.331272 | 0.000000 |
| 1 | -0.034844 | 2.614744 | 0.000000 |

**45P**

| | | | |
|---|---|---|---|
| 7 | 1.607776 | -0.666787 | 0.000000 |
| 15 | 1.539931 | 0.987738 | 0.000000 |
| 7 | 0.000000 | 1.529170 | 0.000000 |
| 15 | -1.453286 | 0.752804 | 0.000000 |
| 15 | -1.144123 | -1.355393 | 0.000000 |
| 6 | 0.612945 | -1.538378 | 0.000000 |
| 1 | 0.930068 | -2.583640 | 0.000000 |

**46P**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 0.000000 | -1.568156 |
| 1 | 0.000000 | 0.000000 | -2.656165 |
| 7 | 0.000000 | 1.358417 | 0.798766 |
| 7 | 0.000000 | -1.358417 | 0.798766 |
| 15 | 0.000000 | 0.000000 | 1.713007 |
| 15 | 0.000000 | 1.574247 | -0.827091 |
| 15 | 0.000000 | -1.574247 | -0.827091 |

Table S14: MP2/cc-pVTZ optimized geometries for the $Li^{+}$-complexed cation-π systems

**1N-π**

| | | | |
|---|---|---|---|
| 3 | 0.002035 | -0.316303 | 1.800284 |
| 6 | 1.156517 | -0.698240 | -0.166374 |
| 6 | 1.201406 | 0.699422 | -0.109898 |
| 6 | -0.003063 | 1.408227 | -0.064184 |
| 6 | -1.204591 | 0.694384 | -0.109599 |
| 6 | -1.153733 | -0.703076 | -0.165770 |
| 1 | 2.065882 | -1.284759 | -0.199006 |
| 1 | 2.152811 | 1.212956 | -0.101055 |
| 1 | -0.005300 | 2.488351 | -0.010627 |
| 1 | -2.158101 | 1.203992 | -0.101379 |
| 1 | -2.060615 | -1.293455 | -0.197909 |
| 7 | 0.002857 | -1.397497 | -0.156560 |

**3N-π**

| | | | |
|---|---|---|---|
| 3 | 0.322970 | -0.000002 | 1.864633 |
| 6 | -0.652416 | 1.190450 | -0.100992 |
| 6 | -1.381788 | 0.000005 | -0.100770 |
| 6 | -0.652426 | -1.190445 | -0.100992 |
| 1 | -1.138679 | 2.156814 | -0.061339 |
| 1 | -2.462295 | 0.000010 | -0.081096 |
| 1 | -1.138697 | -2.156805 | -0.061340 |
| 7 | 0.694276 | 1.198798 | -0.141399 |
| 7 | 0.694267 | -1.198804 | -0.141399 |
| 6 | 1.298849 | -0.000005 | -0.215089 |
| 1 | 2.377644 | -0.000009 | -0.303486 |

**4N-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.000000 | 1.859690 |
| 6 | 1.145458 | 0.700131 | -0.150158 |
| 6 | 1.145458 | -0.700131 | -0.150158 |
| 1 | 2.068905 | 1.265253 | -0.157214 |
| 1 | 2.068905 | -1.265253 | -0.157214 |
| 7 | 0.000000 | -1.406048 | -0.096173 |
| 6 | -1.145458 | -0.700131 | -0.150158 |
| 1 | -2.068905 | -1.265253 | -0.157214 |
| 6 | -1.145458 | 0.700131 | -0.150158 |
| 7 | 0.000000 | 1.406048 | -0.096173 |
| 1 | -2.068905 | 1.265253 | -0.157214 |

**7N-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.000000 | 1.967213 |
| 7 | 0.000000 | 1.376231 | -0.131544 |
| 6 | -1.131537 | 0.653293 | -0.148364 |
| 1 | -2.069278 | 1.194698 | -0.156220 |
| 7 | 1.191851 | -0.688116 | -0.131544 |
| 6 | 0.000000 | -1.306586 | -0.148364 |
| 1 | 0.000000 | -2.389396 | -0.156220 |
| 6 | 1.131537 | 0.653293 | -0.148364 |
| 7 | -1.191851 | -0.688115 | -0.131544 |
| 1 | 2.069278 | 1.194698 | -0.156220 |

**1P-π**

| | | | |
|---|---|---|---|
| 3 | 1.792565 | 0.284260 | 0.000000 |
| 15 | -0.156860 | -1.524741 | 0.000000 |
| 6 | -0.086032 | -0.383794 | 1.328736 |
| 6 | -0.086032 | 1.012328 | 1.227969 |
| 6 | -0.092175 | 1.688629 | 0.000000 |
| 6 | -0.086032 | 1.012328 | -1.227969 |
| 6 | -0.086032 | -0.383794 | -1.328736 |
| 1 | -0.076362 | -0.813323 | 2.324763 |
| 1 | -0.077357 | 1.600154 | 2.138145 |
| 1 | -0.099545 | 2.770493 | 0.000000 |
| 1 | -0.077357 | 1.600154 | -2.138145 |
| 1 | -0.076362 | -0.813323 | -2.324763 |

**2P-π**

| | | | |
|---|---|---|---|
| 3 | 1.826546 | -0.402739 | 0.000000 |
| 6 | -0.040195 | -0.541713 | 1.507267 |
| 6 | -0.040195 | -1.684379 | 0.702042 |
| 6 | -0.040195 | -1.684379 | -0.702042 |
| 6 | -0.040195 | -0.541713 | -1.507267 |
| 1 | 0.001043 | -0.713347 | 2.579613 |
| 1 | -0.020390 | -2.648457 | 1.197120 |
| 1 | -0.020390 | -2.648457 | -1.197120 |
| 1 | 0.001043 | -0.713347 | -2.579613 |
| 15 | -0.149209 | 1.154831 | -1.066838 |
| 15 | -0.149209 | 1.154831 | 1.066838 |

**3P-π**

| | | | |
|---|---|---|---|
| 3 | -1.804573 | 0.309043 | 0.000000 |
| 6 | 0.106366 | 1.060616 | 1.246497 |
| 6 | -0.001204 | -1.334852 | 0.000000 |
| 6 | 0.106366 | 1.060616 | -1.246497 |
| 6 | 0.111152 | 1.700700 | 0.000000 |
| 1 | 0.121855 | 1.705218 | 2.119813 |
| 1 | -0.071906 | -2.421490 | 0.000000 |
| 1 | 0.121855 | 1.705218 | -2.119813 |
| 1 | 0.114838 | 2.786262 | 0.000000 |
| 15 | 0.106366 | -0.654161 | -1.606666 |
| 15 | 0.106366 | -0.654161 | 1.606666 |

**4P-π**

| | | | |
|---|---|---|---|
| 3 | 1.815291 | 0.000000 | 0.000000 |
| 6 | -0.051115 | 1.349282 | 0.698958 |
| 6 | -0.051115 | -1.349283 | 0.698958 |
| 6 | -0.051115 | -1.349283 | -0.698958 |
| 6 | -0.051115 | 1.349282 | -0.698958 |
| 1 | -0.015373 | 2.321979 | 1.183280 |
| 1 | -0.015373 | -2.321978 | 1.183281 |
| 1 | -0.015373 | -2.321978 | -1.183281 |
| 1 | -0.015373 | 2.321979 | -1.183280 |
| 15 | -0.138587 | 0.000000 | -1.817439 |
| 15 | -0.138587 | 0.000000 | 1.817439 |

**5P-π**

| | | | |
|---|---|---|---|
| 3 | 1.800399 | 0.509740 | 0.000000 |
| 6 | -0.090582 | 1.295404 | 1.257184 |
| 6 | -0.108698 | 1.913683 | 0.000000 |
| 6 | -0.090582 | 1.295404 | -1.257184 |
| 1 | -0.091309 | 1.975448 | 2.105740 |
| 1 | -0.122761 | 2.999195 | 0.000000 |
| 1 | -0.091309 | 1.975448 | -2.105740 |
| 15 | -0.090582 | -0.386591 | -1.756466 |
| 15 | -0.042613 | -1.593902 | 0.000000 |
| 15 | -0.090582 | -0.386591 | 1.756466 |

**6P-π**

| | | | |
|---|---|---|---|
| 3 | -0.181389 | 0.189112 | 1.817835 |
| 6 | -1.122331 | 1.339595 | -0.090249 |
| 6 | -0.667451 | -1.359137 | 0.027067 |
| 1 | -1.804315 | 2.186897 | -0.096656 |
| 1 | -1.053026 | -2.374939 | 0.126663 |
| 6 | 0.235870 | 1.661778 | -0.023790 |
| 1 | 0.459094 | 2.724773 | 0.051003 |
| 15 | -1.964077 | -0.200482 | -0.152683 |
| 15 | 1.082530 | -1.353864 | -0.063456 |
| 15 | 1.699273 | 0.690514 | -0.118039 |

**7P-π**

| | | | |
|---|---|---|---|
| 3 | -1.819203 | 0.000000 | 0.000000 |
| 6 | 0.043652 | -1.584270 | 0.000000 |
| 1 | 0.024913 | -2.673891 | 0.000000 |
| 6 | 0.043652 | 0.792135 | 1.372018 |
| 1 | 0.024913 | 1.336945 | 2.315658 |
| 6 | 0.043652 | 0.792135 | -1.372018 |
| 1 | 0.024913 | 1.336945 | -2.315658 |
| 15 | 0.102159 | -0.937701 | -1.624146 |
| 15 | 0.102159 | 1.875402 | 0.000000 |
| 15 | 0.102159 | -0.937701 | 1.624146 |

**8P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.373972 | 1.801393 |
| 6 | 0.699288 | 1.744409 | -0.024669 |
| 6 | -0.699288 | 1.744409 | -0.024669 |
| 1 | 1.148886 | 2.733956 | 0.043430 |
| 1 | -1.148888 | 2.733956 | 0.043430 |
| 15 | 1.946892 | 0.510751 | -0.157501 |
| 15 | 1.065512 | -1.428175 | -0.015666 |
| 15 | -1.065511 | -1.428175 | -0.015666 |
| 15 | -1.946892 | 0.510750 | -0.157501 |

**9P-π**

| | | | |
|---|---|---|---|
| 3 | -0.245641 | 0.000000 | 1.801044 |
| 6 | -1.034832 | 1.388559 | -0.023272 |
| 1 | -1.625388 | 2.305777 | 0.021096 |
| 15 | 0.673082 | -1.785822 | -0.043312 |
| 15 | 1.841314 | 0.000003 | -0.103590 |
| 15 | 0.673075 | 1.785824 | -0.043312 |
| 6 | -1.034826 | -1.388563 | -0.023273 |
| 15 | -2.093761 | -0.000003 | -0.154189 |
| 1 | -1.625380 | -2.305782 | 0.021096 |

**10P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.000000 | 1.834228 |
| 15 | 1.632846 | 1.069268 | -0.136948 |
| 15 | 1.632846 | -1.069268 | -0.136948 |
| 6 | 0.000000 | 1.634658 | 0.158270 |
| 15 | -1.632846 | 1.069268 | -0.136948 |
| 1 | 0.000000 | 2.698088 | 0.407474 |
| 15 | -1.632846 | -1.069268 | -0.136948 |
| 6 | 0.000000 | -1.634658 | 0.158270 |
| 1 | 0.000000 | -2.698088 | 0.407474 |

**11P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.155395 | 1.824775 |
| 15 | -1.628757 | 1.306074 | -0.131561 |
| 15 | -1.775806 | -0.821198 | -0.226394 |
| 6 | 0.000000 | 1.828396 | 0.263786 |
| 15 | 1.628758 | 1.306074 | -0.131561 |
| 1 | 0.000000 | 2.864967 | 0.608453 |
| 15 | 1.775806 | -0.821199 | -0.226394 |
| 15 | 0.000000 | -1.923186 | 0.204878 |

**13-π**

| | | | |
|---|---|---|---|
| 3 | 0.295780 | -0.210275 | 1.827703 |
| 7 | -0.389697 | -1.314921 | -0.066743 |
| 15 | -1.476104 | -0.051550 | -0.107268 |
| 6 | -0.407923 | 1.340938 | -0.048653 |
| 6 | 0.986949 | 1.240592 | -0.089967 |
| 6 | 1.647603 | 0.006889 | -0.177178 |
| 6 | 0.944006 | -1.206557 | -0.166868 |
| 1 | -0.852032 | 2.330030 | 0.001427 |
| 1 | 1.584610 | 2.144447 | -0.064294 |
| 1 | 2.727522 | -0.017355 | -0.239364 |
| 1 | 1.498187 | -2.139784 | -0.208669 |

**14-π**

| | | | |
|---|---|---|---|
| 3 | -0.506635 | -0.282360 | 1.813453 |
| 7 | -0.996247 | -1.235834 | -0.153034 |
| 6 | 0.349819 | -1.290857 | -0.119010 |
| 15 | 1.523167 | 0.020185 | -0.078657 |
| 6 | 0.373837 | 1.337956 | -0.008992 |
| 6 | -1.011027 | 1.201010 | -0.122574 |
| 6 | -1.634255 | -0.051006 | -0.207487 |
| 1 | 0.748493 | -2.301601 | -0.107084 |
| 1 | 0.778036 | 2.340438 | 0.083176 |
| 1 | -1.637902 | 2.084871 | -0.128042 |
| 1 | -2.712738 | -0.111181 | -0.288931 |

**15-π**

| | | | |
|---|---|---|---|
| 3 | 0.293093 | 1.904118 | 0.000000 |
| 7 | -1.562512 | 0.648502 | 0.000000 |
| 6 | -0.966650 | 0.332490 | 1.167502 |
| 6 | 0.293093 | -0.255710 | 1.313173 |
| 15 | 1.327457 | -0.768683 | 0.000000 |
| 6 | 0.293093 | -0.255710 | -1.313173 |
| 6 | -0.966650 | 0.332490 | -1.167502 |
| 1 | -1.535706 | 0.599275 | 2.051688 |
| 1 | 0.650272 | -0.420762 | 2.323872 |
| 1 | 0.650272 | -0.420762 | -2.323872 |
| 1 | -1.535706 | 0.599275 | -2.051688 |

**18N-π**

| | | | |
|---|---|---|---|
| 3 | 0.259193 | 0.000000 | 1.890895 |
| 7 | -0.415247 | 1.323121 | -0.040272 |
| 15 | -1.421750 | 0.000000 | -0.126735 |
| 7 | -0.415245 | -1.323122 | -0.040272 |
| 6 | 0.920315 | -1.220030 | -0.124975 |
| 6 | 1.610538 | 0.000000 | -0.201427 |
| 6 | 0.920314 | 1.220030 | -0.124975 |
| 1 | 1.482881 | -2.149433 | -0.108990 |
| 1 | 2.689355 | 0.000000 | -0.281613 |
| 1 | 1.482879 | 2.149434 | -0.108990 |

**19N-π**

| | | | |
|---|---|---|---|
| 3 | 0.653103 | -0.248594 | 1.867523 |

| | | | |
|---|---|---|---|
| 7 | 1.639694 | 0.025968 | -0.189411 |
| 6 | 0.949227 | -1.129679 | -0.244411 |
| 7 | -0.364458 | -1.305968 | -0.080615 |
| 15 | -1.477719 | -0.067502 | -0.036061 |
| 6 | -0.422155 | 1.326245 | -0.084789 |
| 6 | 0.968488 | 1.193440 | -0.113775 |
| 1 | 1.551237 | -2.022358 | -0.382628 |
| 1 | -0.843700 | 2.325334 | -0.061961 |
| 1 | 1.598923 | 2.075305 | -0.069023 |

**20N-π**

| | | | |
|---|---|---|---|
| 3 | 0.678834 | 0.000000 | 1.854623 |
| 7 | 1.002798 | 1.203684 | -0.139013 |
| 6 | 1.583395 | 0.000000 | -0.272284 |
| 7 | 1.002799 | -1.203684 | -0.139013 |
| 6 | -0.334799 | -1.296809 | -0.038078 |
| 15 | -1.520452 | 0.000000 | -0.082789 |
| 6 | -0.334800 | 1.296809 | -0.038078 |
| 1 | 2.653030 | 0.000000 | -0.441073 |
| 1 | -0.702355 | -2.312736 | 0.077931 |
| 1 | -0.702356 | 2.312735 | 0.077931 |

**21N-π**

| | | | |
|---|---|---|---|
| 3 | 0.475681 | 0.145071 | 1.863294 |
| 7 | -0.378460 | -1.326142 | 0.010212 |
| 15 | -1.473624 | -0.075691 | -0.091611 |
| 6 | -0.368942 | 1.301481 | -0.107655 |
| 7 | 0.977439 | 1.242584 | -0.124660 |
| 6 | 1.599107 | 0.051031 | -0.227797 |
| 6 | 0.944066 | -1.188073 | -0.144884 |
| 1 | -0.774062 | 2.309675 | -0.063218 |
| 1 | 2.678089 | 0.088472 | -0.318856 |
| 1 | 1.535062 | -2.099719 | -0.150492 |

**32-π**

| | | | |
|---|---|---|---|
| 3 | 0.164955 | 0.332249 | 1.909311 |
| 7 | 1.268871 | 0.995370 | -0.086692 |
| 15 | 1.465532 | -0.653442 | -0.164259 |
| 7 | -0.022376 | -1.327797 | 0.074495 |
| 15 | -1.525218 | -0.647411 | -0.070618 |
| 6 | -1.176785 | 1.071887 | -0.192654 |
| 6 | 0.098344 | 1.654556 | -0.108979 |
| 1 | -2.024727 | 1.745840 | -0.268271 |
| 1 | 0.170328 | 2.738531 | -0.041338 |

**33-π**

| | | | |
|---|---|---|---|
| 3 | -1.916751 | -0.158062 | 0.000000 |
| 7 | -0.006599 | -0.719246 | 1.325859 |
| 15 | 0.222554 | -1.697488 | 0.000000 |
| 7 | -0.006599 | -0.719246 | -1.325859 |
| 6 | -0.006599 | 0.618844 | -1.336667 |
| 15 | 0.195412 | 1.762180 | 0.000000 |
| 6 | -0.006599 | 0.618844 | 1.336667 |
| 1 | -0.173830 | 1.073561 | -2.313716 |
| 1 | -0.173830 | 1.073561 | 2.313716 |

**34-π**

| | | | |
|---|---|---|---|
| 3 | -1.184282 | -0.034803 | 1.823726 |
| 7 | -1.263740 | 1.194905 | -0.149471 |
| 6 | -1.663515 | -0.051161 | -0.446363 |
| 7 | -1.020831 | -1.171235 | -0.115903 |
| 15 | 0.632991 | -1.352109 | 0.046196 |
| 15 | 1.499580 | 0.604201 | -0.131690 |
| 6 | 0.010229 | 1.513945 | 0.120216 |
| 1 | -2.656335 | -0.145602 | -0.874785 |
| 1 | 0.132335 | 2.526246 | 0.500522 |

**36-π**

| | | | |
|---|---|---|---|
| 3 | -1.821512 | 0.727451 | 0.000000 |
| 7 | 0.017210 | 0.514763 | 1.483026 |
| 6 | 0.316689 | 1.563327 | 0.703318 |
| 6 | 0.316689 | 1.563327 | -0.703318 |
| 7 | 0.017210 | 0.514763 | -1.483026 |
| 15 | 0.017210 | -1.105830 | -1.088150 |
| 15 | 0.017210 | -1.105830 | 1.088150 |
| 1 | 0.453506 | 2.512971 | 1.214250 |
| 1 | 0.453506 | 2.512971 | -1.214250 |

**37-π**

| | | | |
|---|---|---|---|
| 3 | -1.908742 | 0.567585 | 0.000000 |
| 7 | 0.023816 | 1.697362 | 0.000000 |
| 6 | 0.137727 | 1.056450 | 1.183477 |
| 15 | 0.137727 | -0.682683 | 1.509106 |
| 7 | -0.068656 | -1.318885 | 0.000000 |
| 15 | 0.137727 | -0.682683 | -1.509106 |
| 6 | 0.137727 | 1.056450 | -1.183477 |
| 1 | 0.127791 | 1.725492 | 2.042279 |
| 1 | 0.127791 | 1.725492 | -2.042279 |

**38-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.000000 | 1.913245 |
| 6 | 0.000000 | 1.495930 | 0.136000 |
| 6 | 0.000000 | -1.495930 | 0.136000 |
| 1 | 0.052854 | 2.507527 | 0.539279 |
| 1 | -0.052854 | -2.507527 | 0.539279 |
| 15 | -1.563477 | 0.733997 | -0.295671 |
| 15 | 1.563477 | -0.733997 | -0.295671 |
| 7 | -1.145813 | -0.833176 | 0.029989 |
| 7 | 1.145813 | 0.833176 | 0.029989 |

**16P-π**

| | | | |
|---|---|---|---|
| 3 | -0.597744 | -0.102204 | 1.823942 |
| 7 | -0.771023 | -1.388640 | -0.056411 |
| 15 | 0.888252 | -1.241556 | -0.083038 |
| 15 | 1.347406 | 0.864546 | -0.054486 |
| 6 | -0.265641 | 1.561102 | -0.034532 |
| 6 | -1.509297 | 0.938822 | -0.184465 |
| 6 | -1.714088 | -0.451280 | -0.202995 |
| 1 | -0.285954 | 2.644244 | 0.052251 |
| 1 | -2.391395 | 1.565791 | -0.248274 |
| 1 | -2.732971 | -0.819653 | -0.286098 |

**17P-π**

| | | | |
|---|---|---|---|
| 3 | -0.767537 | -0.126575 | 1.813653 |
| 7 | -1.660117 | -0.746574 | -0.159054 |
| 6 | -0.528008 | -1.467382 | -0.102732 |
| 15 | 1.180979 | -1.030605 | -0.078186 |
| 15 | 1.135515 | 1.098214 | -0.007793 |
| 6 | -0.576195 | 1.463382 | -0.106216 |
| 6 | -1.668880 | 0.600375 | -0.218089 |
| 1 | -0.710003 | -2.540007 | -0.062278 |
| 1 | -0.815382 | 2.523474 | -0.094757 |

| | | | |
|---|---|---|---|
| 1 | -2.660109 | 1.029901 | -0.318648 |

**18P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.214904 | 1.847771 |
| 7 | 0.000000 | -1.305700 | 0.040591 |
| 15 | -1.522577 | -0.683897 | -0.115363 |
| 6 | -1.245354 | 1.053961 | -0.118397 |
| 6 | 0.000000 | 1.701347 | -0.098266 |
| 6 | 1.245354 | 1.053961 | -0.118397 |
| 15 | 1.522576 | -0.683898 | -0.115363 |
| 1 | -2.129546 | 1.684732 | -0.138871 |
| 1 | 0.000000 | 2.787053 | -0.078471 |
| 1 | 2.129547 | 1.684731 | -0.138871 |

**19P-π**

| | | | |
|---|---|---|---|
| 3 | 0.151338 | 0.440255 | 1.840948 |
| 7 | 1.272918 | 1.006420 | -0.092641 |
| 15 | 1.558791 | -0.630004 | -0.126774 |
| 6 | -0.030819 | -1.352444 | 0.014867 |
| 15 | -1.613551 | -0.617773 | -0.068462 |
| 6 | -1.178960 | 1.078897 | -0.146238 |
| 6 | 0.099762 | 1.653559 | -0.149091 |
| 1 | -0.040333 | -2.438158 | 0.102571 |
| 1 | -2.014458 | 1.770196 | -0.192734 |
| 1 | 0.171846 | 2.738840 | -0.172883 |

**20P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.616912 | 1.829729 |
| 7 | 0.000001 | 1.700007 | -0.123136 |
| 6 | 1.185067 | 1.061381 | -0.158771 |
| 15 | 1.592956 | -0.650325 | -0.101355 |
| 6 | 0.000000 | -1.339557 | 0.078962 |
| 15 | -1.592956 | -0.650324 | -0.101355 |
| 6 | -1.185066 | 1.061382 | -0.158770 |
| 1 | 2.035012 | 1.738417 | -0.194500 |
| 1 | -0.000002 | -2.417131 | 0.233890 |
| 1 | -2.035011 | 1.738420 | -0.194499 |

**21P-π**

| | | | |
|---|---|---|---|
| 3 | 0.074293 | -0.189399 | 1.857454 |
| 7 | 0.704338 | -1.327491 | -0.031421 |
| 15 | 1.761067 | -0.048938 | -0.166748 |
| 6 | 0.710145 | 1.357234 | -0.036688 |
| 6 | -0.686278 | 1.357508 | 0.000125 |
| 15 | -1.790739 | -0.000704 | -0.151401 |
| 6 | -0.633624 | -1.333632 | -0.073721 |
| 1 | 1.211345 | 2.321165 | 0.022883 |
| 1 | -1.177128 | 2.323450 | 0.092605 |
| 1 | -1.083822 | -2.326004 | -0.033954 |

**23P-π**

| | | | |
|---|---|---|---|
| 3 | 0.000000 | 0.795274 | 1.835298 |
| 7 | 0.000000 | 1.913082 | -0.097419 |
| 6 | -1.194998 | 1.298611 | -0.144749 |
| 15 | -1.734367 | -0.379197 | -0.124889 |
| 15 | 0.000000 | -1.599787 | 0.065867 |
| 15 | 1.734367 | -0.379198 | -0.124889 |
| 6 | 1.195000 | 1.298610 | -0.144749 |
| 1 | -2.022810 | 2.005995 | -0.164147 |
| 1 | 2.022812 | 2.005993 | -0.164147 |

**24P-π**

| | | | |
|---|---|---|---|
| 3 | -0.224219 | 0.087188 | 1.860342 |
| 7 | -0.714056 | -1.289853 | 0.086186 |
| 15 | 0.928109 | -1.392399 | -0.064012 |
| 15 | 1.729916 | 0.617585 | -0.142528 |
| 6 | 0.306774 | 1.643562 | 0.034806 |
| 6 | -1.059648 | 1.373014 | -0.106121 |
| 15 | -1.901596 | -0.175651 | -0.184085 |
| 1 | 0.564442 | 2.688199 | 0.200906 |
| 1 | -1.722596 | 2.236714 | -0.097972 |

**25P-π**

| | | | |
|---|---|---|---|
| 3 | 0.165283 | -0.388180 | 1.861233 |
| 7 | -0.191633 | -1.642695 | 0.040674 |
| 15 | -1.599575 | -0.773816 | -0.139503 |
| 15 | -1.128585 | 1.334805 | -0.080423 |
| 6 | 0.609905 | 1.368381 | 0.127214 |
| 15 | 1.920212 | 0.247801 | -0.181493 |
| 6 | 1.092380 | -1.313321 | -0.135023 |
| 1 | 0.979703 | 2.367912 | 0.358370 |
| 1 | 1.771385 | -2.166699 | -0.158656 |

**26P-π**

| | | | |
|---|---|---|---|
| 3 | 0.285442 | -0.252413 | 1.872013 |
| 7 | 1.063597 | -1.326043 | -0.031516 |
| 15 | 1.902121 | 0.089383 | -0.255044 |
| 6 | 0.728907 | 1.341128 | 0.107043 |
| 15 | -1.018100 | 1.369516 | -0.021164 |
| 15 | -1.685697 | -0.653000 | -0.198167 |
| 6 | -0.229242 | -1.625687 | 0.073211 |
| 1 | 1.157105 | 2.324695 | 0.303807 |
| 1 | -0.431447 | -2.666275 | 0.334852 |

**27P-π**

| | | | |
|---|---|---|---|
| 3 | -0.094934 | 0.000000 | 1.857100 |
| 7 | -1.546720 | 0.000004 | -0.000108 |
| 15 | -0.965352 | -1.537549 | -0.118758 |
| 6 | 0.782422 | -1.373146 | -0.059932 |
| 15 | 1.871014 | -0.000005 | -0.078533 |
| 6 | 0.782429 | 1.373142 | -0.059931 |
| 15 | -0.965343 | 1.537554 | -0.118758 |
| 1 | 1.308971 | -2.327944 | -0.055314 |
| 1 | 1.308984 | 2.327937 | -0.055314 |

**39P-π**

| | | | |
|---|---|---|---|
| 7 | 0.266766 | 1.652325 | 0.128867 |
| 15 | 1.613918 | 0.946318 | -0.443752 |
| 15 | 1.413933 | -1.125830 | 0.203840 |
| 15 | -0.643928 | -1.497328 | -0.118666 |
| 15 | -1.982921 | 0.140615 | -0.313157 |
| 6 | -1.014425 | 1.473310 | 0.370872 |
| 1 | -1.518101 | 2.234683 | 0.968912 |
| 3 | -0.092584 | 0.134185 | 1.993270 |

**40P-π**

| | | | |
|---|---|---|---|
| 7 | -0.829995 | -1.327295 | -0.056736 |
| 15 | -1.956067 | -0.202279 | -0.459329 |

| | | | |
|---|---|---|---|
| 6 | -1.197394 | 1.232649 | 0.227611 |
| 15 | 0.489378 | 1.707013 | 0.129836 |
| 15 | 1.834280 | 0.160484 | -0.389120 |
| 15 | 0.759187 | -1.622956 | 0.227208 |
| 1 | -1.850924 | 2.051208 | 0.529355 |
| 3 | -0.685470 | -0.263328 | 1.957735 |

**41P-π**

| | | | |
|---|---|---|---|
| 7 | 0.248709 | -1.588002 | 0.000000 |
| 15 | -0.174017 | -1.086587 | 1.519391 |
| 15 | -0.174017 | 1.075009 | 1.588444 |
| 6 | 0.344655 | 1.598509 | 0.000000 |
| 15 | -0.174017 | 1.075009 | -1.588444 |
| 15 | -0.174017 | -1.086587 | -1.519391 |
| 1 | 0.874678 | 2.552206 | 0.000000 |
| 3 | 1.919147 | -0.226633 | 0.000000 |

Table S15: MP2/cc-pVTZ optimized geometries for the $Li^+$-complexed cation-σ systems.

**1N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.192274 | 0.000000 |
| 6 | 1.154526 | 0.493338 | 0.000000 |
| 6 | 1.196207 | -0.893661 | 0.000000 |
| 6 | 0.000000 | -1.603153 | 0.000000 |
| 6 | -1.196207 | -0.893661 | 0.000000 |
| 6 | -1.154526 | 0.493338 | 0.000000 |
| 1 | 2.072170 | 1.067563 | 0.000000 |
| 1 | 2.150488 | -1.399007 | 0.000000 |
| 1 | 0.000000 | -2.683929 | 0.000000 |
| 1 | -2.150489 | -1.399007 | 0.000000 |
| 1 | -2.072169 | 1.067563 | 0.000000 |
| 3 | 0.000000 | 3.141234 | 0.000000 |

**2N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | -0.138709 | 1.343256 | 0.000000 |
| 6 | -1.370842 | 0.692647 | 0.000000 |
| 6 | -1.370842 | -0.692647 | 0.000000 |
| 6 | -0.138710 | -1.343255 | 0.000000 |
| 1 | -0.049957 | 2.419950 | 0.000000 |
| 1 | -2.288667 | 1.261691 | 0.000000 |
| 1 | -2.288667 | -1.261692 | 0.000000 |
| 1 | -0.049957 | -2.419950 | 0.000000 |
| 7 | 1.015341 | 0.671821 | 0.000000 |
| 7 | 1.015342 | -0.671821 | 0.000000 |
| 3 | 2.859028 | 0.000000 | 0.000000 |

**3N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | -0.056951 | -1.557581 | 0.000000 |
| 6 | -1.132525 | 0.436870 | 0.000000 |
| 6 | 1.157884 | 0.477036 | 0.000000 |
| 6 | 1.172637 | -0.907208 | 0.000000 |
| 1 | -0.124953 | -2.637156 | 0.000000 |
| 1 | -2.069782 | 0.979448 | 0.000000 |
| 1 | 2.077605 | 1.046577 | 0.000000 |
| 1 | 2.104083 | -1.452264 | 0.000000 |
| 7 | 0.000000 | 1.168540 | 0.000000 |
| 7 | -1.214030 | -0.886056 | 0.000000 |
| 3 | -0.111671 | 3.130437 | 0.000000 |

**4N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | -1.145438 | -0.470418 |
| 6 | 0.000000 | 1.145438 | -0.470418 |
| 6 | 0.000000 | 1.134491 | 0.920826 |
| 6 | 0.000000 | -1.134491 | 0.920826 |
| 1 | 0.000000 | -2.079050 | -1.016747 |
| 1 | 0.000000 | 2.079050 | -1.016747 |
| 1 | 0.000000 | 2.063123 | 1.475113 |
| 1 | 0.000000 | -2.063123 | 1.475113 |
| 7 | 0.000000 | 0.000000 | -1.181124 |
| 7 | 0.000000 | 0.000000 | 1.627680 |
| 3 | 0.000000 | 0.000000 | -3.149176 |

**5N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.209279 | 0.669435 | 0.000000 |
| 6 | -1.025449 | -0.890881 | 0.000000 |
| 6 | 0.216447 | -1.507432 | 0.000000 |
| 6 | 1.322883 | -0.668049 | 0.000000 |
| 1 | -1.960137 | -1.432922 | 0.000000 |
| 1 | 0.316923 | -2.582489 | 0.000000 |
| 1 | 2.336866 | -1.041500 | 0.000000 |
| 7 | 0.000000 | 1.183976 | 0.000000 |
| 7 | -1.113539 | 0.443636 | 0.000000 |
| 3 | -1.482373 | 2.458584 | 0.000000 |

**6N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | -1.009487 | -0.877279 | 0.000000 |
| 6 | 0.252481 | -1.478977 | 0.000000 |
| 1 | -1.932602 | -1.438339 | 0.000000 |
| 1 | 0.363465 | -2.554949 | 0.000000 |
| 7 | 0.000000 | 1.193918 | 0.000000 |
| 7 | -1.118223 | 0.450455 | 0.000000 |
| 3 | -1.586649 | 2.382068 | 0.000000 |
| 6 | 1.184118 | 0.579040 | 0.000000 |
| 7 | 1.362513 | -0.745314 | 0.000000 |
| 1 | 2.056387 | 1.216962 | 0.000000 |

**7N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.187573 | -0.903901 |
| 6 | 0.000000 | 0.000000 | -1.517509 |
| 1 | 0.000000 | 0.000000 | -2.598772 |
| 7 | 0.000000 | -1.187573 | -0.903901 |
| 7 | 0.000000 | 0.000000 | 1.147997 |
| 6 | 0.000000 | -1.133205 | 0.418495 |
| 1 | 0.000000 | -2.075491 | 0.952162 |
| 6 | 0.000000 | 1.133205 | 0.418495 |
| 1 | 0.000000 | 2.075491 | 0.952162 |
| 3 | 0.000000 | 0.000000 | 3.132066 |

**8N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 6 | -1.295602 | 0.697617 | 0.000000 |
| 6 | -1.295602 | -0.697617 | 0.000000 |
| 1 | -2.204090 | 1.283335 | 0.000000 |
| 1 | -2.204090 | -1.283335 | 0.000000 |
| 7 | -0.150448 | 1.384860 | 0.000000 |
| 7 | 0.958374 | 0.665330 | 0.000000 |
| 7 | 0.958374 | -0.665331 | 0.000000 |
| 7 | -0.150448 | -1.384860 | 0.000000 |
| 3 | 2.881480 | 0.000000 | 0.000000 |

**9N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 6 | -0.253271 | 1.301445 | 0.000049 |
| 1 | -0.270211 | 2.382385 | 0.000045 |
| 1 | -2.167546 | -1.299351 | 0.000575 |
| 7 | -0.104408 | -1.358777 | 0.000129 |
| 7 | 0.983755 | -0.627559 | -0.000037 |
| 7 | 0.945315 | 0.706000 | 0.000013 |
| 7 | -1.403026 | 0.633207 | 0.000020 |
| 6 | -1.273653 | -0.691888 | -0.000278 |
| 3 | 2.882617 | -0.070159 | -0.000039 |

**10N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 1 | -0.205836 | -2.365622 | 0.000000 |
| 1 | -0.205837 | 2.365623 | 0.000000 |
| 7 | 0.979382 | 0.668875 | 0.000000 |

| | | | |
|---|---|---|---|
| 7 | 0.979382 | -0.668875 | 0.000000 |
| 7 | -1.392685 | 0.662652 | 0.000000 |
| 6 | -0.203902 | 1.285395 | 0.000000 |
| 7 | -1.392685 | -0.662652 | 0.000000 |
| 6 | -0.203902 | -1.285395 | 0.000000 |
| 3 | 2.881585 | 0.000000 | 0.000000 |

**11N–$\sigma'_{3aN}$**

| | | | |
|---|---|---|---|
| 1 | -0.000001 | -2.554686 | 0.000000 |
| 7 | 1.171256 | 0.462146 | 0.000000 |
| 7 | 1.187697 | -0.857108 | 0.000000 |
| 7 | -1.171256 | 0.462147 | 0.000000 |
| 7 | -1.187697 | -0.857108 | 0.000000 |
| 6 | 0.000000 | -1.474040 | 0.000000 |
| 7 | 0.000000 | 1.086204 | 0.000000 |
| 3 | 0.000000 | 3.108319 | 0.000000 |

**13–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.213245 | 0.000000 |
| 15 | -1.350224 | 0.215783 | 0.000000 |
| 6 | -0.670454 | -1.375517 | 0.000000 |
| 6 | 0.698891 | -1.612264 | 0.000000 |
| 6 | 1.634818 | -0.578273 | 0.000000 |
| 6 | 1.266743 | 0.762494 | 0.000000 |
| 1 | -1.357451 | -2.213528 | 0.000000 |
| 1 | 1.057293 | -2.634036 | 0.000000 |
| 1 | 2.689296 | -0.814419 | 0.000000 |
| 1 | 2.050842 | 1.512093 | 0.000000 |
| 3 | -0.588866 | 3.080597 | 0.000000 |

**14–$\sigma'_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.240321 | 0.685561 | 0.000000 |
| 6 | 0.000000 | 1.218161 | 0.000000 |
| 15 | -1.546261 | 0.413576 | 0.000000 |
| 6 | -0.965018 | -1.224093 | 0.000000 |
| 6 | 0.375576 | -1.583390 | 0.000000 |
| 6 | 1.407144 | -0.649540 | 0.000000 |
| 1 | -0.030404 | 2.304607 | 0.000000 |
| 1 | -1.706403 | -2.014559 | 0.000000 |
| 1 | 0.650359 | -2.630154 | 0.000000 |
| 1 | 2.431149 | -1.000977 | 0.000000 |
| 3 | 2.753589 | 1.923898 | 0.000000 |

**15–$\sigma'_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.167034 | -0.830961 |
| 6 | 0.000000 | -1.167034 | -0.830961 |
| 6 | 0.000000 | -1.309440 | 0.546718 |
| 6 | 0.000000 | 1.309440 | 0.546718 |
| 1 | 0.000000 | 2.060715 | -1.445731 |
| 1 | 0.000000 | -2.060715 | -1.445731 |
| 1 | 0.000000 | -2.320093 | 0.935521 |
| 1 | 0.000000 | 2.320093 | 0.935521 |
| 7 | 0.000000 | 0.000000 | -1.507528 |
| 15 | 0.000000 | 0.000000 | 1.690941 |
| 3 | 0.000000 | 0.000000 | -3.460027 |

**16N–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.250221 | 0.712106 | 0.000000 |
| 7 | 0.000000 | 1.201736 | 0.000000 |
| 15 | -1.433155 | 0.342392 | 0.000000 |
| 6 | -0.838173 | -1.296722 | 0.000000 |
| 6 | 0.514019 | -1.595998 | 0.000000 |
| 6 | 1.494319 | -0.599389 | 0.000000 |
| 1 | -1.557747 | -2.107329 | 0.000000 |
| 1 | 0.842847 | -2.627271 | 0.000000 |
| 1 | 2.544074 | -0.857866 | 0.000000 |
| 3 | 1.298540 | 2.670779 | 0.000000 |

**17N– $\sigma''_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.408230 | -0.584412 | 0.000000 |
| 7 | 1.212730 | 0.741548 | 0.000000 |
| 6 | 0.000000 | 1.297146 | 0.000000 |
| 15 | -1.563020 | 0.506186 | 0.000000 |
| 6 | -0.956194 | -1.120034 | 0.000000 |
| 6 | 0.392290 | -1.454188 | 0.000000 |
| 1 | 0.030214 | 2.380806 | 0.000000 |
| 1 | -1.671052 | -1.934034 | 0.000000 |
| 1 | 0.704887 | -2.490477 | 0.000000 |
| 3 | 3.139316 | 0.337805 | 0.000000 |

**18N–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.217342 | 0.000000 |
| 15 | -1.314276 | 0.165411 | 0.000000 |
| 7 | -0.712591 | -1.349036 | 0.000000 |
| 6 | 0.595831 | -1.601102 | 0.000000 |
| 6 | 1.583404 | -0.613219 | 0.000000 |
| 6 | 1.259464 | 0.738835 | 0.000000 |
| 1 | 0.889035 | -2.645906 | 0.000000 |
| 1 | 2.624955 | -0.899316 | 0.000000 |
| 1 | 2.067458 | 1.463040 | 0.000000 |
| 3 | -0.503789 | 3.125262 | 0.000000 |

**19N–$\sigma'_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.225980 | 0.806881 | 0.000000 |
| 6 | 0.000000 | 1.377670 | 0.000000 |
| 7 | -1.176646 | 0.790940 | 0.000000 |
| 15 | -1.396256 | -0.848682 | 0.000000 |
| 6 | 0.249092 | -1.416816 | 0.000000 |
| 6 | 1.320855 | -0.539356 | 0.000000 |
| 1 | -0.002947 | 2.465136 | 0.000000 |
| 1 | 0.460967 | -2.478894 | 0.000000 |
| 1 | 2.330663 | -0.935820 | 0.000000 |
| 3 | 2.796712 | 1.988689 | 0.000000 |

**20N–$\sigma'_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.376338 | -1.593782 | 0.000000 |
| 6 | 1.343491 | -0.685230 | 0.000000 |
| 7 | 1.226492 | 0.654515 | 0.000000 |
| 6 | 0.000000 | 1.215152 | 0.000000 |
| 15 | -1.543443 | 0.411714 | 0.000000 |
| 6 | -0.902223 | -1.214618 | 0.000000 |
| 1 | 2.353316 | -1.078360 | 0.000000 |
| 1 | -0.009331 | 2.301454 | 0.000000 |
| 1 | -1.614211 | -2.034496 | 0.000000 |
| 3 | 2.851486 | 1.772912 | 0.000000 |

**21N–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.204720 | 0.000000 |
| 15 | -1.350123 | 0.203986 | 0.000000 |
| 6 | -0.604873 | -1.375253 | 0.000000 |
| 7 | 0.702256 | -1.638032 | 0.000000 |
| 6 | 1.581690 | -0.628801 | 0.000000 |

| | | | |
|---|---|---|---|
| 6 | 1.256299 | 0.726729 | 0.000000 |
| 1 | -1.258498 | -2.242844 | 0.000000 |
| 1 | 2.626494 | -0.911948 | 0.000000 |
| 1 | 2.065913 | 1.448865 | 0.000000 |
| 3 | -0.498850 | 3.114424 | 0.000000 |

**22N–σ′′$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.532891 | -0.602722 | 0.000000 |
| 7 | -1.238411 | 0.675232 | 0.000000 |
| 7 | 0.000000 | 1.178422 | 0.000000 |
| 15 | 1.445152 | 0.331008 | 0.000000 |
| 6 | 0.809969 | -1.285379 | 0.000000 |
| 6 | -0.556098 | -1.529187 | 0.000000 |
| 1 | 1.487798 | -2.130868 | 0.000000 |
| 1 | -0.934258 | -2.543704 | 0.000000 |
| 3 | -1.451645 | 2.613441 | 0.000000 |

**23N–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.390721 | -1.494032 | 0.000000 |
| 7 | 1.366508 | -0.610468 | 0.000000 |
| 7 | 1.198503 | 0.716791 | 0.000000 |
| 6 | 0.000000 | 1.304953 | 0.000000 |
| 15 | -1.555184 | 0.511676 | 0.000000 |
| 6 | -0.889676 | -1.106859 | 0.000000 |
| 1 | 0.047928 | 2.388134 | 0.000000 |
| 1 | -1.577745 | -1.945241 | 0.000000 |
| 3 | 3.168504 | 0.135789 | 0.000000 |

**24N–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.243929 | 0.696764 | 0.000000 |
| 7 | 0.000000 | 1.207004 | 0.000000 |
| 15 | -1.400427 | 0.289058 | 0.000000 |
| 7 | -0.869838 | -1.275378 | 0.000000 |
| 6 | 0.418848 | -1.577737 | 0.000000 |
| 6 | 1.449858 | -0.620901 | 0.000000 |
| 1 | 0.687443 | -2.629711 | 0.000000 |
| 1 | 2.487868 | -0.923209 | 0.000000 |
| 3 | 1.333410 | 2.670047 | 0.000000 |

**25N–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.193036 | 0.000000 |
| 7 | 1.240099 | 0.677258 | 0.000000 |
| 6 | 1.445120 | -0.639987 | 0.000000 |
| 7 | 0.524318 | -1.611253 | 0.000000 |
| 6 | -0.767749 | -1.299054 | 0.000000 |
| 15 | -1.430666 | 0.330037 | 0.000000 |
| 1 | 2.482886 | -0.944037 | 0.000000 |
| 1 | -1.448445 | -2.145776 | 0.000000 |
| 3 | 1.336801 | 2.653410 | 0.000000 |

**26N–σ′′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.203336 | 0.737486 | 0.000000 |
| 7 | 1.359280 | -0.594742 | 0.000000 |
| 6 | 0.309575 | -1.427681 | 0.000000 |
| 7 | -0.975443 | -1.106171 | 0.000000 |
| 15 | -1.532366 | 0.445763 | 0.000000 |
| 6 | 0.000000 | 1.314387 | 0.000000 |
| 1 | 0.574964 | -2.478698 | 0.000000 |
| 1 | 0.035963 | 2.398465 | 0.000000 |
| 3 | 3.135633 | 0.272516 | 0.000000 |

**27N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 0.000000 | 1.575732 |
| 7 | 0.000000 | 0.000000 | -1.429274 |
| 3 | 0.000000 | 0.000000 | -3.406308 |
| 7 | 0.000000 | 1.315168 | 0.574896 |
| 7 | 0.000000 | -1.315168 | 0.574896 |
| 6 | 0.000000 | 1.160304 | -0.732520 |
| 6 | 0.000000 | -1.160304 | -0.732520 |
| 1 | 0.000000 | 2.065334 | -1.335218 |
| 1 | 0.000000 | -2.065334 | -1.335218 |

**28–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.291525 | 1.090595 | 0.000000 |
| 7 | 0.000000 | 1.440091 | 0.000000 |
| 15 | -1.394715 | 0.517813 | 0.000000 |
| 15 | -0.785941 | -1.532247 | 0.000000 |
| 6 | 0.943898 | -1.339169 | 0.000000 |
| 6 | 1.713649 | -0.178834 | 0.000000 |
| 1 | 1.510876 | -2.265189 | 0.000000 |
| 1 | 2.793307 | -0.262502 | 0.000000 |
| 3 | 1.139901 | 3.045807 | 0.000000 |

**29–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.103796 | -1.560640 | 0.000000 |
| 7 | -1.103554 | -0.980272 | 0.000000 |
| 15 | -1.521128 | 0.638589 | 0.000000 |
| 6 | 0.000000 | 1.475503 | 0.000000 |
| 15 | 1.608779 | 0.832672 | 0.000000 |
| 6 | 1.257330 | -0.890145 | 0.000000 |
| 1 | -0.069951 | 2.561257 | 0.000000 |
| 1 | 2.115789 | -1.553623 | 0.000000 |
| 3 | -1.302094 | -2.934105 | 0.000000 |

**30–σ′′$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.191944 | -0.671684 | 0.000000 |
| 15 | 0.095023 | 1.735642 | 0.000000 |
| 6 | 1.501758 | 0.691821 | 0.000000 |
| 6 | 1.501758 | -0.691821 | 0.000000 |
| 1 | 2.460533 | 1.203324 | 0.000000 |
| 1 | 2.460534 | -1.203324 | 0.000000 |
| 15 | 0.095023 | -1.735641 | 0.000000 |
| 7 | -1.191944 | 0.671683 | 0.000000 |
| 3 | -3.035216 | 0.000000 | 0.000000 |

**31–σ′′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.533007 | -0.669320 | 0.000000 |
| 7 | 1.533007 | 0.669321 | 0.000000 |
| 6 | 0.436936 | 1.431159 | 0.000000 |
| 15 | -1.274370 | 1.060480 | 0.000000 |
| 15 | -1.274369 | -1.060480 | 0.000000 |
| 6 | 0.436936 | -1.431158 | 0.000000 |
| 1 | 0.685447 | 2.488572 | 0.000000 |
| 1 | 0.685448 | -2.488571 | 0.000000 |
| 3 | 3.384945 | 0.000000 | 0.000000 |

**32–σ′$_{3bN}$**

| | | | |
|---|---|---|---|
| 7 | -1.250095 | -1.186025 | 0.000000 |
| 15 | -1.481406 | 0.421944 | 0.000000 |
| 7 | 0.000000 | 1.203159 | 0.000000 |

| | | | |
|---|---|---|---|
| 15 | 1.506424 | 0.474193 | 0.000000 |
| 6 | 1.180355 | -1.226363 | 0.000000 |
| 6 | -0.081118 | -1.825307 | 0.000000 |
| 1 | 2.049773 | -1.874477 | 0.000000 |
| 1 | -0.138406 | -2.910773 | 0.000000 |
| 3 | -0.043800 | 3.177759 | 0.000000 |

**33–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | -1.250422 | -1.012097 | 0.000000 |
| 15 | -1.494446 | 0.600441 | 0.000000 |
| 7 | 0.000000 | 1.372560 | 0.000000 |
| 6 | 1.181851 | 0.730346 | 0.000000 |
| 15 | 1.544852 | -0.982325 | 0.000000 |
| 6 | -0.084826 | -1.643682 | 0.000000 |
| 1 | 2.065063 | 1.368362 | 0.000000 |
| 1 | -0.146313 | -2.731397 | 0.000000 |
| 3 | -0.168018 | 3.349357 | 0.000000 |

**34–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.406676 | -1.794815 | 0.000000 |
| 6 | 1.411014 | -0.919750 | 0.000000 |
| 7 | 1.376829 | 0.413919 | 0.000000 |
| 15 | 0.000000 | 1.384917 | 0.000000 |
| 15 | -1.688202 | 0.118793 | 0.000000 |
| 6 | -0.874461 | -1.440151 | 0.000000 |
| 1 | 2.395756 | -1.376145 | 0.000000 |
| 1 | -1.552520 | -2.291066 | 0.000000 |
| 3 | 2.925317 | 1.645743 | 0.000000 |

**35–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | -1.599387 | -0.354971 | 0.000000 |
| 6 | -1.236729 | 0.909250 | 0.000000 |
| 7 | 0.000000 | 1.445593 | 0.000000 |
| 15 | 1.437212 | 0.584115 | 0.000000 |
| 6 | 0.990917 | -1.077053 | 0.000000 |
| 15 | -0.636441 | -1.693940 | 0.000000 |
| 1 | -2.055254 | 1.627463 | 0.000000 |
| 1 | 1.809361 | -1.792451 | 0.000000 |
| 3 | 0.301637 | 3.394940 | 0.000000 |

**36–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | -0.941584 | -1.444159 | 0.000000 |
| 6 | 0.346133 | -1.773330 | 0.000000 |
| 6 | 1.437294 | -0.898542 | 0.000000 |
| 7 | 1.377908 | 0.441243 | 0.000000 |
| 15 | 0.000000 | 1.408168 | 0.000000 |
| 15 | -1.661295 | 0.030460 | 0.000000 |
| 1 | 0.564950 | -2.837190 | 0.000000 |
| 1 | 2.429321 | -1.337536 | 0.000000 |
| 3 | 2.723441 | 1.882316 | 0.000000 |

**37–σ′$_{3aN}$**

| | | | |
|---|---|---|---|
| 6 | -1.170014 | 1.244821 | 0.000000 |
| 1 | -2.042706 | 1.894053 | 0.000000 |
| 7 | 0.000000 | -1.188402 | 0.000000 |
| 7 | 0.000000 | 1.890453 | 0.000000 |
| 15 | -1.511393 | -0.471293 | 0.000000 |
| 15 | 1.511393 | -0.471292 | 0.000000 |
| 6 | 1.170014 | 1.244821 | 0.000000 |
| 1 | 2.042706 | 1.894053 | 0.000000 |
| 3 | 0.000000 | -3.167183 | 0.000000 |

**38–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | 1.191013 | 0.741314 | 0.000000 |
| 6 | -1.152803 | -1.088137 | 0.000000 |
| 1 | 2.065591 | 1.392624 | 0.000000 |
| 1 | -2.024003 | -1.744495 | 0.000000 |
| 15 | 1.524159 | -0.986045 | 0.000000 |
| 15 | -1.510751 | 0.630589 | 0.000000 |
| 7 | 0.026613 | -1.688066 | 0.000000 |
| 7 | 0.000000 | 1.368002 | 0.000000 |
| 3 | -0.219424 | 3.335033 | 0.000000 |

**39N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | 0.358739 | -1.509832 | 0.000000 |
| 7 | 1.328555 | -0.610430 | 0.000000 |
| 7 | 1.157308 | 0.715801 | 0.000000 |
| 7 | 0.000000 | 1.331264 | 0.000000 |
| 15 | -1.481421 | 0.553543 | 0.000000 |
| 6 | -0.917405 | -1.112184 | 0.000000 |
| 1 | -1.622206 | -1.937812 | 0.000000 |
| 3 | 3.145245 | 0.273384 | 0.000000 |

**40N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -0.840404 | -1.267145 | 0.000000 |
| 6 | 0.458236 | -1.516098 | 0.000000 |
| 7 | 1.480300 | -0.626211 | 0.000000 |
| 7 | 1.227357 | 0.658405 | 0.000000 |
| 7 | 0.000000 | 1.189394 | 0.000000 |
| 15 | -1.408503 | 0.277553 | 0.000000 |
| 1 | 0.783431 | -2.550136 | 0.000000 |
| 3 | 1.507974 | 2.600773 | 0.000000 |

**41N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | -0.821653 | -1.290066 | 0.000000 |
| 7 | 0.457035 | -1.620282 | 0.000000 |
| 6 | 1.396434 | -0.655489 | 0.000000 |
| 7 | 1.226832 | 0.671476 | 0.000000 |
| 7 | 0.000000 | 1.210031 | 0.000000 |
| 15 | -1.398589 | 0.276558 | 0.000000 |
| 1 | 2.421448 | -0.998542 | 0.000000 |
| 3 | 1.381093 | 2.661665 | 0.000000 |

**42N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 15 | -0.762255 | -1.526706 | 0.000000 |
| 15 | -1.410214 | 0.508322 | 0.000000 |
| 7 | 0.000000 | 1.407975 | 0.000000 |
| 7 | 1.288343 | 1.054156 | 0.000000 |
| 7 | 1.754670 | -0.174271 | 0.000000 |
| 6 | 0.970607 | -1.261464 | 0.000000 |
| 1 | 1.569924 | -2.167850 | 0.000000 |
| 3 | 1.297460 | 2.999124 | 0.000000 |

**43N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.435487 | 0.000000 |
| 7 | -1.232034 | 0.916027 | 0.000000 |
| 7 | -1.525861 | -0.352941 | 0.000000 |
| 15 | -0.495578 | -1.678753 | 0.000000 |
| 6 | 1.104885 | -0.999678 | 0.000000 |
| 15 | 1.502585 | 0.687441 | 0.000000 |

| | | | |
|---|---|---|---|
| 1 | 1.939731 | -1.697502 | 0.000000 |
| 3 | -1.456291 | 2.858416 | 0.000000 |

**44N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.419300 | 0.000000 |
| 7 | 1.283190 | 1.031803 | 0.000000 |
| 15 | -1.418867 | 0.526843 | 0.000000 |
| 3 | 1.182138 | 3.006653 | 0.000000 |
| 15 | -0.704383 | -1.518572 | 0.000000 |
| 7 | 0.933049 | -1.347220 | 0.000000 |
| 6 | 1.673039 | -0.249510 | 0.000000 |
| 1 | 2.750428 | -0.374147 | 0.000000 |

**45N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.101489 | -1.562360 | 0.000000 |
| 7 | -1.102456 | -0.965289 | 0.000000 |
| 15 | 1.522062 | 0.864299 | 0.000000 |
| 7 | 0.000000 | 1.460160 | 0.000000 |
| 6 | 1.256068 | -0.889679 | 0.000000 |
| 15 | -1.434753 | 0.678589 | 0.000000 |
| 1 | 2.122115 | -1.544514 | 0.000000 |
| 3 | -1.320465 | -2.929431 | 0.000000 |

**46N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 6 | 1.262251 | -1.014466 | 0.000000 |
| 1 | 2.148504 | -1.650360 | 0.000000 |
| 7 | 0.000000 | 1.363747 | 0.000000 |
| 7 | -1.174331 | 0.706880 | 0.000000 |
| 7 | 0.101115 | -1.642998 | 0.000000 |
| 15 | -1.400779 | -0.951016 | 0.000000 |
| 15 | 1.550721 | 0.735482 | 0.000000 |
| 3 | -1.486210 | 2.658923 | 0.000000 |

**47N–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | 1.241569 | 0.898707 | 0.000000 |
| 1 | 2.066402 | 1.610628 | 0.000000 |
| 7 | -0.994001 | -1.062627 | 0.000000 |
| 7 | 0.000000 | 1.438628 | 0.000000 |
| 15 | -1.395555 | 0.501878 | 0.000000 |
| 3 | -0.298554 | 3.398893 | 0.000000 |
| 15 | 0.544089 | -1.650223 | 0.000000 |
| 7 | 1.587122 | -0.372339 | 0.000000 |

Table S16: MP2/cc-pVTZ optimized geometries for the P-analogues $Li^{+}$-complexed cation-σ systems

**1P–σ′$_{1P}$**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 1.219554 | 0.000000 |
| 6 | -1.361763 | 0.164834 | 0.000000 |
| 6 | -1.229577 | -1.220489 | 0.000000 |
| 6 | 0.000000 | -1.880291 | 0.000000 |
| 6 | 1.229577 | -1.220489 | 0.000000 |
| 6 | 1.361762 | 0.164834 | 0.000000 |
| 1 | -2.352694 | 0.600614 | 0.000000 |
| 1 | -2.131792 | -1.818227 | 0.000000 |
| 1 | 0.000000 | -2.961518 | 0.000000 |
| 1 | 2.131792 | -1.818227 | 0.000000 |
| 1 | 2.352693 | 0.600614 | 0.000000 |
| 3 | 0.000000 | 3.684349 | 0.000000 |

**2P–σ′$_{2aP}$**

| | | | |
|---|---|---|---|
| 6 | -0.664249 | -1.615942 | 0.000000 |
| 6 | 0.705457 | -1.852586 | 0.000000 |
| 6 | 1.718874 | -0.888099 | 0.000000 |
| 6 | 1.533260 | 0.488196 | 0.000000 |
| 1 | -1.304905 | -2.492596 | 0.000000 |
| 1 | 1.023057 | -2.888301 | 0.000000 |
| 1 | 2.740182 | -1.248503 | 0.000000 |
| 1 | 2.414919 | 1.119057 | 0.000000 |
| 15 | 0.000000 | 1.288397 | 0.000000 |
| 15 | -1.554337 | -0.116543 | 0.000000 |
| 3 | -0.439416 | 3.714373 | 0.000000 |

**3P–σ′$_{1P}$**

| | | | |
|---|---|---|---|
| 6 | 0.912384 | -1.322309 | 0.000000 |
| 6 | 0.000000 | 1.300909 | 0.000000 |
| 6 | -1.540419 | -0.938991 | 0.000000 |
| 6 | -0.411852 | -1.756189 | 0.000000 |
| 1 | 1.694830 | -2.071436 | 0.000000 |
| 1 | 0.162012 | 2.374748 | 0.000000 |
| 1 | -2.499193 | -1.446682 | 0.000000 |
| 1 | -0.574176 | -2.828350 | 0.000000 |
| 15 | -1.664943 | 0.799104 | 0.000000 |
| 15 | 1.412087 | 0.324971 | 0.000000 |
| 3 | 3.749566 | 1.136697 | 0.000000 |

**4P–σ′$_{1P}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.387332 | -0.504791 |
| 6 | 0.000000 | -1.387332 | -0.504791 |
| 6 | 0.000000 | -1.362825 | 0.883090 |
| 6 | 0.000000 | 1.362825 | 0.883090 |
| 1 | 0.000000 | 2.352021 | -1.001730 |
| 1 | 0.000000 | -2.352021 | -1.001730 |
| 1 | 0.000000 | -2.328037 | 1.380931 |
| 1 | 0.000000 | 2.328037 | 1.380931 |
| 15 | 0.000000 | 0.000000 | 1.976322 |
| 15 | 0.000000 | 0.000000 | -1.529806 |
| 3 | 0.000000 | 0.000000 | -3.998583 |

**5P–σ′$_{3aP}$**

| | | | |
|---|---|---|---|
| 6 | 1.258570 | -1.453476 | 0.000000 |
| 6 | 0.000000 | -2.053081 | 0.000000 |
| 6 | -1.258570 | -1.453476 | 0.000000 |
| 1 | 2.099674 | -2.141816 | 0.000000 |
| 1 | 0.000000 | -3.137933 | 0.000000 |
| 1 | -2.099674 | -2.141816 | 0.000000 |
| 15 | -1.785010 | 0.205869 | 0.000000 |
| 15 | 0.000000 | 1.311421 | 0.000000 |
| 15 | 1.785010 | 0.205868 | 0.000000 |
| 3 | 0.000000 | 3.778134 | 0.000000 |

**6P–σ′$_{2aP}$**

| | | | |
|---|---|---|---|
| 6 | -0.050801 | -1.892474 | 0.000000 |
| 6 | -1.431424 | 0.496325 | 0.000000 |
| 1 | -0.067164 | -2.979573 | 0.000000 |
| 1 | -2.358619 | 1.065174 | 0.000000 |
| 6 | 1.215136 | -1.323115 | 0.000000 |
| 1 | 2.047918 | -2.022893 | 0.000000 |
| 15 | -1.666015 | -1.224860 | 0.000000 |
| 15 | 0.000000 | 1.456958 | 0.000000 |
| 15 | 1.768752 | 0.332607 | 0.000000 |
| 3 | 0.146445 | 3.927434 | 0.000000 |

**7P–σ′$_{1P}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.411045 | 0.627588 |
| 6 | 0.000000 | 0.000000 | -1.735543 |
| 6 | 0.000000 | -1.411045 | 0.627588 |
| 1 | 0.000000 | 2.344312 | 1.184586 |
| 1 | 0.000000 | 0.000000 | -2.824915 |
| 1 | 0.000000 | -2.344312 | 1.184586 |
| 15 | 0.000000 | 1.617638 | -1.100709 |
| 15 | 0.000000 | -1.617638 | -1.100709 |
| 15 | 0.000000 | 0.000000 | 1.606350 |
| 3 | 0.000000 | 0.000000 | 4.087988 |

**8P–σ′$_{3bP}$**

| | | | |
|---|---|---|---|
| 6 | 1.641909 | -1.108692 | 0.000000 |
| 6 | 0.523129 | -1.934646 | 0.000000 |
| 1 | 2.594649 | -1.634947 | 0.000000 |
| 1 | 0.756706 | -2.998238 | 0.000000 |
| 15 | 1.904184 | 0.615706 | 0.000000 |
| 15 | 0.000000 | 1.505833 | 0.000000 |
| 15 | -1.735082 | 0.334450 | 0.000000 |
| 15 | -1.210306 | -1.723345 | 0.000000 |
| 3 | -0.241176 | 3.967851 | 0.000000 |

**9P–σ′$_{3aP}$**

| | | | |
|---|---|---|---|
| 6 | -1.403990 | 1.178553 | 0.000000 |
| 1 | -2.313963 | 1.781082 | 0.000000 |
| 15 | 1.817886 | -0.509413 | 0.000000 |
| 15 | 0.000000 | -1.564359 | 0.000000 |
| 15 | -1.817886 | -0.509413 | 0.000000 |
| 6 | 1.403990 | 1.178553 | 0.000000 |
| 15 | 0.000000 | 2.210041 | 0.000000 |
| 1 | 2.313963 | 1.781083 | 0.000000 |
| 3 | 0.000000 | -4.035877 | 0.000000 |

**10P–σ′$_{2aP}$**

| | | | |
|---|---|---|---|
| 15 | 1.503294 | 0.789534 | 0.000000 |
| 15 | 1.402382 | -1.307531 | 0.000000 |
| 6 | 0.000000 | 1.633739 | 0.000000 |
| 15 | -1.674577 | 1.161450 | 0.000000 |

| | | | |
|---|---|---|---|
| 1 | 0.122202 | 2.716581 | 0.000000 |
| 15 | -1.852075 | -0.962589 | 0.000000 |
| 6 | -0.285193 | -1.723022 | 0.000000 |
| 1 | -0.395137 | -2.809542 | 0.000000 |
| 3 | 3.766245 | 1.805229 | 0.000000 |

**11P–σ′$_{3aP}$**

| | | | |
|---|---|---|---|
| 15 | 1.433109 | 1.661416 | 0.000000 |
| 15 | -0.683094 | 1.857738 | 0.000000 |
| 6 | 1.957467 | 0.000000 | 0.000000 |
| 15 | 1.433109 | -1.661415 | 0.000000 |
| 15 | -0.683095 | -1.857738 | 0.000000 |
| 1 | 3.051175 | 0.000000 | 0.000000 |
| 15 | -1.658979 | 0.000000 | 0.000000 |
| 3 | -4.137241 | 0.000000 | 0.000000 |

**16P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | 1.490303 | -0.886663 | 0.000000 |
| 6 | -0.925772 | -1.453491 | 0.000000 |
| 6 | 0.424438 | -1.786576 | 0.000000 |
| 1 | 2.494619 | -1.296713 | 0.000000 |
| 1 | -1.621287 | -2.287721 | 0.000000 |
| 1 | 0.686016 | -2.837314 | 0.000000 |
| 15 | -1.695789 | 0.109865 | 0.000000 |
| 15 | 0.000000 | 1.378040 | 0.000000 |
| 7 | 1.400729 | 0.447430 | 0.000000 |
| 3 | 2.712856 | 1.910516 | 0.000000 |

**17P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.292288 | 1.058145 | 0.000000 |
| 6 | 0.000000 | 1.437696 | 0.000000 |
| 15 | -1.503554 | 0.553743 | 0.000000 |
| 15 | -0.891819 | -1.473354 | 0.000000 |
| 6 | 0.846244 | -1.355913 | 0.000000 |
| 6 | 1.664406 | -0.236793 | 0.000000 |
| 1 | -0.138117 | 2.518650 | 0.000000 |
| 1 | 1.368393 | -2.307728 | 0.000000 |
| 1 | 2.737095 | -0.399596 | 0.000000 |
| 3 | 2.617769 | 2.501964 | 0.000000 |

**18P–σ′$_{3aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.187811 | 0.000000 |
| 15 | -1.516984 | 0.489740 | 0.000000 |
| 6 | -1.234850 | -1.220485 | 0.000000 |
| 6 | 0.000000 | -1.865985 | 0.000000 |
| 6 | 1.234850 | -1.220486 | 0.000000 |
| 15 | 1.516984 | 0.489740 | 0.000000 |
| 1 | -2.129269 | -1.834624 | 0.000000 |
| 1 | 0.000000 | -2.950651 | 0.000000 |
| 1 | 2.129269 | -1.834624 | 0.000000 |
| 3 | 0.000000 | 3.151582 | 0.000000 |

**19P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.017341 | -1.083124 | 0.000000 |
| 15 | 1.461194 | 0.531178 | 0.000000 |
| 6 | 0.000000 | 1.443538 | 0.000000 |
| 15 | -1.644300 | 0.888052 | 0.000000 |
| 6 | -1.417756 | -0.840472 | 0.000000 |
| 6 | -0.236359 | -1.569025 | 0.000000 |
| 1 | 0.139337 | 2.521863 | 0.000000 |
| 1 | -2.329993 | -1.426057 | 0.000000 |
| 1 | -0.319277 | -2.652415 | 0.000000 |
| 3 | 2.686608 | -2.118074 | 0.000000 |

**20P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.232485 | 0.946851 | 0.000000 |
| 6 | 0.000000 | 1.491404 | 0.000000 |
| 15 | -1.589303 | 0.766511 | 0.000000 |
| 6 | -1.197712 | -0.920137 | 0.000000 |
| 15 | 0.331054 | -1.733155 | 0.000000 |
| 6 | 1.441031 | -0.384339 | 0.000000 |
| 1 | -0.007116 | 2.578696 | 0.000000 |
| 1 | -2.060159 | -1.582708 | 0.000000 |
| 1 | 2.489764 | -0.671411 | 0.000000 |
| 3 | 2.787977 | 2.141852 | 0.000000 |

**21P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.368175 | 0.000000 |
| 15 | -1.519453 | 0.662018 | 0.000000 |
| 6 | -1.231372 | -1.051290 | 0.000000 |
| 6 | -0.000209 | -1.686617 | 0.000000 |
| 15 | 1.587572 | -0.962557 | 0.000000 |
| 6 | 1.187364 | 0.738348 | 0.000000 |
| 1 | -2.128386 | -1.664318 | 0.000000 |
| 1 | -0.002546 | -2.772824 | 0.000000 |
| 1 | 2.057448 | 1.393735 | 0.000000 |
| 3 | -0.227671 | 3.323873 | 0.000000 |

**22P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.482184 | 0.799809 | 0.000000 |
| 15 | 0.000000 | 1.583402 | 0.000000 |
| 15 | -1.662057 | 0.285925 | 0.000000 |
| 15 | -0.872575 | -1.679962 | 0.000000 |
| 6 | 0.870632 | -1.575105 | 0.000000 |
| 6 | 1.762980 | -0.509019 | 0.000000 |
| 1 | 1.342062 | -2.553900 | 0.000000 |
| 1 | 2.821188 | -0.753561 | 0.000000 |
| 3 | 2.559759 | 2.457690 | 0.000000 |

**23P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | -1.783222 | 0.000000 |
| 6 | 1.193027 | -1.159874 | 0.000000 |
| 15 | 1.715365 | 0.506508 | 0.000000 |
| 15 | 0.000000 | 1.743395 | 0.000000 |
| 15 | -1.715365 | 0.506508 | 0.000000 |
| 6 | -1.193028 | -1.159873 | 0.000000 |
| 1 | 2.037486 | -1.848138 | 0.000000 |
| 1 | -2.037487 | -1.848137 | 0.000000 |
| 3 | 0.000000 | -3.749615 | 0.000000 |

**24P–σ′$_{3bN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.393283 | 0.000000 |
| 15 | -1.455058 | 0.566053 | 0.000000 |
| 15 | -1.152926 | -1.536914 | 0.000000 |
| 6 | 0.584159 | -1.726654 | 0.000000 |
| 6 | 1.620492 | -0.802591 | 0.000000 |
| 15 | 1.599969 | 0.939657 | 0.000000 |
| 1 | 0.885088 | -2.771970 | 0.000000 |
| 1 | 2.630357 | -1.206344 | 0.000000 |
| 3 | -0.541037 | 3.289620 | 0.000000 |

**25P–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.557467 | 0.000000 |
| 15 | -1.464546 | 0.737636 | 0.000000 |
| 15 | -1.199536 | -1.373183 | 0.000000 |
| 6 | 0.524203 | -1.566857 | 0.000000 |
| 15 | 1.919219 | -0.526807 | 0.000000 |
| 6 | 1.255495 | 1.093589 | 0.000000 |
| 1 | 0.811798 | -2.618698 | 0.000000 |
| 1 | 2.022009 | 1.867368 | 0.000000 |
| 3 | -0.779686 | 3.374659 | 0.000000 |

**26P–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.232250 | 1.038643 | 0.000000 |
| 15 | 1.710656 | -0.565661 | 0.000000 |
| 6 | 0.296424 | -1.556469 | 0.000000 |
| 15 | -1.410155 | -1.229597 | 0.000000 |
| 15 | -1.611738 | 0.888597 | 0.000000 |
| 6 | 0.000000 | 1.566870 | 0.000000 |
| 1 | 0.539401 | -2.619269 | 0.000000 |
| 1 | -0.020002 | 2.657628 | 0.000000 |
| 3 | 2.914953 | 2.076219 | 0.000000 |

**27P–$\sigma'_{3aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.449969 | 0.000000 |
| 15 | 1.530404 | 0.789430 | 0.000000 |
| 6 | 1.366718 | -0.928347 | 0.000000 |
| 15 | 0.000000 | -2.004413 | 0.000000 |
| 6 | -1.366718 | -0.928348 | 0.000000 |
| 15 | -1.530404 | 0.789429 | 0.000000 |
| 1 | 2.328152 | -1.439230 | 0.000000 |
| 1 | -2.328152 | -1.439230 | 0.000000 |
| 3 | 0.000000 | 3.417382 | 0.000000 |

**39P–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.763960 | 0.000000 |
| 15 | -1.497050 | 1.009148 | 0.000000 |
| 15 | -1.477709 | -1.110071 | 0.000000 |
| 15 | 0.512344 | -1.818822 | 0.000000 |
| 15 | 1.987897 | -0.282756 | 0.000000 |
| 6 | 1.256056 | 1.307798 | 0.000000 |
| 1 | 2.011694 | 2.093732 | 0.000000 |
| 3 | -0.810086 | 3.583089 | 0.000000 |

**40P–$\sigma'_{3bN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.612681 | 0.000000 |
| 15 | 1.599336 | 1.158862 | 0.000000 |
| 6 | 1.675185 | -0.573429 | 0.000000 |
| 15 | 0.583336 | -1.930140 | 0.000000 |
| 15 | -1.431702 | -1.253729 | 0.000000 |
| 15 | -1.490756 | 0.859931 | 0.000000 |
| 1 | 2.714457 | -0.907211 | 0.000000 |
| 3 | -0.556259 | 3.511723 | 0.000000 |

**41P–$\sigma'_{3aN}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 0.000000 | -1.790515 |
| 1 | 0.000000 | 0.000000 | -2.882276 |
| 15 | 0.000000 | 1.633957 | -1.194624 |
| 15 | 0.000000 | 1.562077 | 0.940725 |
| 15 | 0.000000 | -1.562077 | 0.940725 |
| 7 | 0.000000 | 0.000000 | 1.531053 |
| 15 | 0.000000 | -1.633957 | -1.194624 |
| 3 | 0.000000 | 0.000000 | 3.508328 |

**42P–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.276927 | 1.269244 | 0.000000 |
| 7 | 0.000000 | 1.659824 | 0.000000 |
| 15 | -1.459418 | 0.838876 | 0.000000 |
| 15 | -1.168667 | -1.271240 | 0.000000 |
| 15 | 0.929210 | -1.578489 | 0.000000 |
| 6 | 1.698834 | 0.000786 | 0.000000 |
| 1 | 2.784665 | -0.047991 | 0.000000 |
| 3 | 1.188988 | 3.234198 | 0.000000 |

**44P–$\sigma''_{3N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.546252 | 0.000000 |
| 7 | 1.240508 | 1.039622 | 0.000000 |
| 15 | 1.795943 | -0.535892 | 0.000000 |
| 6 | 0.391760 | -1.568646 | 0.000000 |
| 15 | -1.325933 | -1.306101 | 0.000000 |
| 15 | -1.513841 | 0.837140 | 0.000000 |
| 1 | 0.661763 | -2.625537 | 0.000000 |
| 3 | 1.320533 | 3.003031 | 0.000000 |

**45P–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.230207 | 1.019568 | 0.000000 |
| 15 | 1.634181 | -0.615911 | 0.000000 |
| 7 | 0.309720 | -1.532811 | 0.000000 |
| 15 | -1.307778 | -1.248181 | 0.000000 |
| 15 | -1.620149 | 0.878841 | 0.000000 |
| 6 | 0.000000 | 1.557690 | 0.000000 |
| 1 | -0.016126 | 2.648942 | 0.000000 |
| 3 | 2.880941 | 2.125454 | 0.000000 |

**46P–$\sigma'_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | 1.348755 | -0.943463 | 0.000000 |
| 1 | 2.293793 | -1.483763 | 0.000000 |
| 7 | 0.000000 | 1.446818 | 0.000000 |
| 7 | -1.354719 | -0.899564 | 0.000000 |
| 15 | -1.497813 | 0.703298 | 0.000000 |
| 15 | 1.531038 | 0.771826 | 0.000000 |
| 15 | -0.084528 | -1.938657 | 0.000000 |
| 3 | -0.044580 | 3.422248 | 0.000000 |

Table S17: MP2/cc-pVTZ optimized geometries for the $Mg^{2+}$-complexed cation-π systems.

**1N-π**

| | | | |
|---|---|---|---|
| 12 | -1.542419 | -0.242030 | 0.000000 |
| 6 | 0.457753 | -0.660070 | 1.171496 |
| 6 | 0.457753 | 0.748002 | 1.214406 |
| 6 | 0.420197 | 1.461326 | 0.000000 |
| 6 | 0.457753 | 0.748002 | -1.214406 |
| 6 | 0.457753 | -0.660070 | -1.171496 |
| 1 | 0.475747 | -1.260153 | 2.075624 |
| 1 | 0.480547 | 1.265879 | 2.166596 |
| 1 | 0.399215 | 2.545299 | 0.000000 |
| 1 | 0.480547 | 1.265879 | -2.166596 |
| 1 | 0.475747 | -1.260153 | -2.075624 |
| 7 | 0.384280 | -1.353646 | 0.000000 |

**3N-π**

| | | | |
|---|---|---|---|
| 12 | -1.560152 | -0.292827 | 0.000000 |
| 6 | 0.414643 | 0.721783 | 1.197566 |
| 6 | 0.477285 | 1.455964 | 0.000000 |
| 6 | 0.414643 | 0.721783 | -1.197566 |
| 1 | 0.347800 | 1.202108 | 2.168797 |
| 1 | 0.509833 | 2.539700 | 0.000000 |
| 1 | 0.347800 | 1.202108 | -2.168797 |
| 7 | 0.414643 | -0.638654 | 1.199649 |
| 7 | 0.414643 | -0.638654 | -1.199649 |
| 6 | 0.536228 | -1.258018 | 0.000000 |
| 1 | 0.654591 | -2.337905 | 0.000000 |

**4N-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.553090 |
| 6 | 1.161820 | 0.704972 | -0.482388 |
| 6 | 1.161820 | -0.704972 | -0.482388 |
| 1 | 2.079591 | 1.285198 | -0.496094 |
| 1 | 2.079591 | -1.285198 | -0.496094 |
| 7 | 0.000000 | -1.399227 | -0.362528 |
| 6 | -1.161820 | -0.704972 | -0.482388 |
| 1 | -2.079591 | -1.285198 | -0.496094 |
| 6 | -1.161820 | 0.704972 | -0.482388 |
| 7 | 0.000000 | 1.399227 | -0.362528 |
| 1 | -2.079591 | 1.285198 | -0.496094 |

**7N-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.555732 |
| 7 | 0.000000 | 1.387630 | -0.425603 |
| 6 | -1.147957 | 0.662773 | -0.464066 |
| 1 | -2.089879 | 1.206592 | -0.459311 |
| 7 | 1.201723 | -0.693815 | -0.425603 |
| 6 | 0.000000 | -1.325546 | -0.464066 |
| 1 | 0.000000 | -2.413184 | -0.459311 |
| 6 | 1.147957 | 0.662773 | -0.464066 |
| 7 | -1.201723 | -0.693815 | -0.425603 |
| 1 | 2.089879 | 1.206592 | -0.459311 |

**1P-π**

| | | | |
|---|---|---|---|
| 12 | 1.573882 | 0.167633 | 0.000000 |
| 15 | -0.468565 | -1.572070 | 0.000000 |
| 6 | -0.337282 | -0.405513 | 1.332664 |
| 6 | -0.337282 | 1.003482 | 1.236047 |
| 6 | -0.347219 | 1.685778 | 0.000000 |
| 6 | -0.337282 | 1.003482 | -1.236047 |
| 6 | -0.337282 | -0.405513 | -1.332664 |
| 1 | -0.327800 | -0.834045 | 2.332134 |
| 1 | -0.329912 | 1.588746 | 2.150581 |
| 1 | -0.364602 | 2.769763 | 0.000000 |
| 1 | -0.329912 | 1.588746 | -2.150581 |
| 1 | -0.327800 | -0.834045 | -2.332134 |

**2P-π**

| | | | |
|---|---|---|---|
| 12 | 1.618112 | -0.210648 | 0.000000 |
| 6 | -0.232722 | -0.525427 | 1.512749 |
| 6 | -0.232722 | -1.681047 | 0.706466 |
| 6 | -0.232722 | -1.681047 | -0.706466 |
| 6 | -0.232722 | -0.525427 | -1.512749 |
| 1 | -0.164266 | -0.694147 | 2.586880 |
| 1 | -0.203090 | -2.644666 | 1.206379 |
| 1 | -0.203090 | -2.644666 | -1.206379 |
| 1 | -0.164266 | -0.694147 | -2.586880 |
| 15 | -0.436577 | 1.189437 | -1.087390 |
| 15 | -0.436577 | 1.189437 | 1.087390 |

**3P-π**

| | | | |
|---|---|---|---|
| 12 | -1.592388 | 0.250042 | 0.000000 |
| 6 | 0.351199 | 1.031697 | 1.255381 |
| 6 | 0.161583 | -1.357592 | 0.000000 |
| 6 | 0.351199 | 1.031697 | -1.255381 |
| 6 | 0.363865 | 1.679108 | 0.000000 |
| 1 | 0.387586 | 1.680477 | 2.127956 |
| 1 | 0.046418 | -2.443431 | 0.000000 |
| 1 | 0.387586 | 1.680477 | -2.127956 |
| 1 | 0.384011 | 2.766359 | 0.000000 |
| 15 | 0.351199 | -0.699794 | -1.635681 |
| 15 | 0.351199 | -0.699794 | 1.635681 |

**4P-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.607246 |
| 6 | 1.351079 | 0.705748 | -0.261057 |
| 6 | -1.351079 | 0.705748 | -0.261057 |
| 6 | -1.351079 | -0.705748 | -0.261057 |
| 6 | 1.351079 | -0.705748 | -0.261057 |
| 1 | 2.328035 | 1.185989 | -0.215674 |
| 1 | -2.328035 | 1.185989 | -0.215674 |
| 1 | -2.328035 | -1.185989 | -0.215674 |
| 1 | 2.328035 | -1.185989 | -0.215674 |
| 15 | 0.000000 | -1.849344 | -0.405296 |
| 15 | 0.000000 | 1.849344 | -0.405296 |

**5P-π**

| | | | |
|---|---|---|---|
| 12 | 1.595681 | 0.374506 | 0.000000 |
| 6 | -0.303264 | 1.263042 | 1.265311 |
| 6 | -0.337972 | 1.887847 | 0.000000 |
| 6 | -0.303264 | 1.263042 | -1.265311 |
| 1 | -0.306814 | 1.946854 | 2.114130 |
| 1 | -0.368310 | 2.974869 | 0.000000 |
| 1 | -0.306814 | 1.946854 | -2.114130 |
| 15 | -0.303264 | -0.432423 | -1.790808 |
| 15 | -0.226754 | -1.658235 | 0.000000 |
| 15 | -0.303264 | -0.432423 | 1.790808 |

**6P-π**

| | | | |
|---|---|---|---|
| 12 | -0.162536 | 0.199662 | 1.610050 |
| 6 | -1.116048 | 1.311894 | -0.366628 |
| 6 | -0.650855 | -1.372713 | -0.080504 |
| 1 | -1.796471 | 2.161513 | -0.425557 |
| 1 | -1.034331 | -2.380695 | 0.102206 |
| 6 | 0.249260 | 1.643110 | -0.245859 |
| 1 | 0.463914 | 2.709712 | -0.162836 |
| 15 | -1.970741 | -0.243450 | -0.427396 |
| 15 | 1.121666 | -1.396265 | -0.207379 |
| 15 | 1.743953 | 0.681033 | -0.343657 |

**7P-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.607578 |
| 6 | 0.000000 | -1.585251 | -0.221101 |
| 1 | 0.000000 | -2.677674 | -0.195583 |
| 6 | 1.372867 | 0.792625 | -0.221101 |
| 1 | 2.318933 | 1.338837 | -0.195583 |
| 6 | -1.372867 | 0.792625 | -0.221101 |
| 1 | -2.318933 | 1.338837 | -0.195583 |
| 15 | -1.652462 | -0.954050 | -0.327208 |
| 15 | 0.000000 | 1.908099 | -0.327208 |
| 15 | 1.652462 | -0.954049 | -0.327208 |

**8P-π**

| | | | |
|---|---|---|---|
| 12 | -1.531072 | 0.563138 | 0.000000 |
| 6 | 0.492687 | 1.660020 | 0.705763 |
| 6 | 0.492687 | 1.660020 | -0.705763 |
| 1 | 0.567146 | 2.652503 | 1.154140 |
| 1 | 0.567146 | 2.652503 | -1.154140 |
| 15 | 0.492687 | 0.409212 | 1.972525 |
| 15 | -0.115143 | -1.475309 | 1.086337 |
| 15 | -0.115143 | -1.475309 | -1.086337 |
| 15 | 0.492687 | 0.409212 | -1.972525 |

**9P-π**

| | | | |
|---|---|---|---|
| 12 | -1.592141 | 0.221471 | 0.000000 |
| 6 | 0.199805 | 1.018951 | 1.388123 |
| 1 | 0.144808 | 1.611662 | 2.306999 |
| 15 | 0.199805 | -0.705930 | -1.818152 |
| 15 | 0.259732 | -1.892243 | 0.000000 |
| 15 | 0.199805 | -0.705930 | 1.818152 |
| 6 | 0.199805 | 1.018951 | -1.388123 |
| 15 | 0.435219 | 2.096877 | 0.000000 |
| 1 | 0.144808 | 1.611662 | -2.306999 |

**10P-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.658407 |
| 15 | 1.650420 | 1.086410 | -0.346648 |
| 15 | 1.650420 | -1.086410 | -0.346648 |
| 6 | 0.000000 | 1.628087 | 0.021770 |
| 15 | -1.650420 | 1.086410 | -0.346648 |
| 1 | 0.000000 | 2.682302 | 0.318376 |
| 15 | -1.650420 | -1.086410 | -0.346648 |
| 6 | 0.000000 | -1.628087 | 0.021770 |
| 1 | 0.000000 | -2.682302 | 0.318376 |

**11P-π**

| | | | |
|---|---|---|---|
| 12 | -1.613442 | -0.153758 | 0.000000 |
| 15 | 0.357386 | -1.312832 | 1.651911 |
| 15 | 0.357386 | 0.851331 | 1.802493 |
| 6 | -0.042128 | -1.834026 | 0.000000 |
| 15 | 0.357386 | -1.312832 | -1.651911 |
| 1 | -0.353605 | -2.884260 | 0.000000 |
| 15 | 0.357386 | 0.851331 | -1.802493 |
| 15 | -0.098367 | 1.971903 | 0.000000 |

**13-π**

| | | | |
|---|---|---|---|
| 12 | 0.298333 | -0.412452 | 1.528032 |
| 7 | -0.382144 | -1.234268 | -0.450617 |
| 15 | -1.553892 | -0.024673 | -0.307824 |
| 6 | -0.499418 | 1.382598 | -0.055903 |
| 6 | 0.904128 | 1.350914 | -0.203710 |
| 6 | 1.603374 | 0.178701 | -0.567423 |
| 6 | 0.943828 | -1.062735 | -0.681935 |
| 1 | -0.964296 | 2.336410 | 0.186644 |
| 1 | 1.471255 | 2.265570 | -0.056674 |
| 1 | 2.674587 | 0.223731 | -0.730841 |
| 1 | 1.510383 | -1.963183 | -0.910015 |

**14-π**

| | | | |
|---|---|---|---|
| 12 | -0.606073 | -0.426663 | 1.452510 |
| 7 | -0.925926 | -1.070430 | -0.692405 |
| 6 | 0.416527 | -1.214739 | -0.514327 |
| 15 | 1.648602 | 0.017091 | -0.143918 |
| 6 | 0.504582 | 1.358568 | 0.045677 |
| 6 | -0.854216 | 1.345557 | -0.324169 |
| 6 | -1.509957 | 0.155725 | -0.701311 |
| 1 | 0.756977 | -2.245612 | -0.600952 |
| 1 | 0.921931 | 2.304049 | 0.384918 |
| 1 | -1.431067 | 2.265013 | -0.284126 |
| 1 | -2.564130 | 0.162483 | -0.959563 |

**15-π**

| | | | |
|---|---|---|---|
| 12 | -1.592600 | -0.365414 | 0.000000 |
| 7 | 0.309354 | -1.645173 | 0.000000 |
| 6 | 0.371798 | -0.975668 | 1.181637 |
| 6 | 0.371798 | 0.426331 | 1.320425 |
| 15 | 0.435292 | 1.604546 | 0.000000 |
| 6 | 0.371798 | 0.426331 | -1.320425 |
| 6 | 0.371798 | -0.975668 | -1.181637 |
| 1 | 0.374368 | -1.611285 | 2.063437 |
| 1 | 0.372218 | 0.823801 | 2.332921 |
| 1 | 0.372218 | 0.823801 | -2.332921 |
| 1 | 0.374368 | -1.611285 | -2.063437 |

**18N-π**

| | | | |
|---|---|---|---|
| 12 | 1.633820 | -0.073047 | 0.000000 |
| 7 | -0.285587 | -0.389953 | 1.308230 |
| 15 | -0.608759 | -1.401178 | 0.000000 |
| 7 | -0.285587 | -0.389953 | -1.308230 |
| 6 | -0.285587 | 0.965054 | -1.221623 |
| 6 | -0.385058 | 1.666888 | 0.000000 |
| 6 | -0.285587 | 0.965054 | 1.221623 |
| 1 | -0.156979 | 1.510388 | -2.154896 |
| 1 | -0.424875 | 2.750825 | 0.000000 |
| 1 | -0.156979 | 1.510388 | 2.154896 |

**19N-π**

| | | | |
|---|---|---|---|
| 12 | 0.913525 | -0.654706 | 1.285474 |
| 7 | 1.374212 | 0.604526 | -0.620898 |
| 6 | 0.911168 | -0.596347 | -1.037849 |
| 7 | -0.224229 | -1.172556 | -0.588519 |
| 15 | -1.568757 | -0.314820 | -0.013117 |
| 6 | -0.860611 | 1.298628 | 0.110036 |
| 6 | 0.522063 | 1.495221 | -0.041405 |
| 1 | 1.566410 | -1.181034 | -1.681038 |
| 1 | -1.474425 | 2.135773 | 0.435336 |
| 1 | 0.991461 | 2.415240 | 0.297995 |

**20N-π**

| | | | |
|---|---|---|---|
| 12 | -1.628440 | -0.442931 | 0.000000 |
| 7 | 0.288354 | -0.947372 | 1.197574 |
| 6 | 0.464957 | -1.550413 | 0.000000 |
| 7 | 0.288354 | -0.947372 | -1.197574 |
| 6 | 0.288354 | 0.408168 | -1.292086 |
| 15 | 0.558904 | 1.603333 | 0.000000 |
| 6 | 0.288354 | 0.408168 | 1.292086 |
| 1 | 0.636919 | -2.622382 | 0.000000 |
| 1 | 0.116918 | 0.777623 | -2.302496 |
| 1 | 0.116918 | 0.777623 | 2.302496 |

**21N-π**

| | | | |
|---|---|---|---|
| 12 | 0.551585 | 0.110112 | 1.528893 |
| 7 | -0.413841 | -1.310477 | -0.064094 |
| 15 | -1.593506 | -0.109555 | -0.178846 |
| 6 | -0.489624 | 1.286424 | -0.359436 |
| 7 | 0.861476 | 1.221334 | -0.500684 |
| 6 | 1.476930 | 0.036112 | -0.759362 |
| 6 | 0.857040 | -1.209521 | -0.521208 |
| 1 | -0.877861 | 2.300543 | -0.260300 |
| 1 | 2.526770 | 0.097723 | -1.030804 |
| 1 | 1.435131 | -2.130383 | -0.579434 |

**32-π**

| | | | |
|---|---|---|---|
| 12 | 0.541532 | -0.127236 | 1.674036 |
| 7 | 1.059939 | 1.102077 | -0.296706 |
| 15 | 1.371635 | -0.463724 | -0.791073 |
| 7 | 0.057352 | -1.271241 | -0.124539 |
| 15 | -1.553244 | -0.719625 | -0.146235 |
| 6 | -1.374686 | 1.023071 | -0.380605 |
| 6 | -0.152359 | 1.669952 | -0.105028 |
| 1 | -2.281810 | 1.619002 | -0.460593 |
| 1 | -0.151224 | 2.684074 | 0.294304 |

**33-π**

| | | | |
|---|---|---|---|
| 12 | -1.693158 | -0.289848 | 0.000000 |
| 7 | 0.149109 | -0.674686 | 1.291093 |
| 15 | 0.576688 | -1.665695 | 0.000000 |
| 7 | 0.149109 | -0.674686 | -1.291093 |
| 6 | 0.149109 | 0.679229 | -1.311760 |
| 15 | 0.541816 | 1.833814 | 0.000000 |
| 6 | 0.149109 | 0.679229 | 1.311760 |
| 1 | -0.168246 | 1.125621 | -2.257502 |
| 1 | -0.168246 | 1.125621 | 2.257502 |

**34-π**

| | | | |
|---|---|---|---|
| 12 | -1.373597 | -0.034149 | 1.265540 |
| 7 | -0.867330 | 1.312634 | -0.571310 |
| 6 | -1.269450 | 0.155856 | -1.120689 |
| 7 | -0.902045 | -1.033494 | -0.595686 |
| 15 | 0.651622 | -1.402100 | -0.009335 |
| 15 | 1.771305 | 0.474951 | 0.034651 |
| 6 | 0.300506 | 1.472270 | 0.095484 |
| 1 | -2.026739 | 0.187712 | -1.901222 |
| 1 | 0.365282 | 2.406582 | 0.655202 |

**35-π**

| | | | |
|---|---|---|---|
| 12 | 1.641413 | -1.146726 | 0.000000 |
| 7 | -0.204506 | -0.860194 | 1.167728 |
| 6 | -0.649426 | -1.354513 | 0.000000 |
| 7 | -0.204506 | -0.860194 | -1.167728 |
| 15 | -0.204506 | 0.819388 | -1.511162 |
| 6 | -0.734141 | 1.508087 | 0.000000 |
| 15 | -0.204506 | 0.819388 | 1.511162 |
| 1 | -1.296594 | -2.234727 | 0.000000 |
| 1 | -1.100704 | 2.535091 | 0.000000 |

**36-π**

| | | | |
|---|---|---|---|
| 12 | 1.695418 | 0.177747 | 0.000000 |
| 7 | 0.092558 | -0.453010 | 1.451552 |
| 6 | 0.092558 | -1.593355 | 0.704606 |
| 6 | 0.092558 | -1.593355 | -0.704606 |
| 7 | 0.092558 | -0.453010 | -1.451552 |
| 15 | -0.781327 | 0.945124 | -1.106480 |
| 15 | -0.781327 | 0.945124 | 1.106480 |
| 1 | 0.344146 | -2.512149 | 1.232056 |
| 1 | 0.344146 | -2.512149 | -1.232056 |

**37-π**

| | | | |
|---|---|---|---|
| 12 | -1.645518 | 0.323197 | 0.000000 |
| 7 | 0.184541 | 1.642591 | 0.000000 |
| 6 | 0.419221 | 1.023174 | 1.191403 |
| 15 | 0.419221 | -0.733413 | 1.527102 |
| 7 | 0.008489 | -1.293726 | 0.000000 |
| 15 | 0.419221 | -0.733413 | -1.527102 |
| 6 | 0.419221 | 1.023174 | -1.191403 |
| 1 | 0.393862 | 1.701938 | 2.045798 |
| 1 | 0.393862 | 1.701938 | -2.045798 |

**38-π**

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 1.691270 |
| 6 | 0.000000 | 1.506328 | -0.098241 |
| 6 | 0.000000 | -1.506328 | -0.098241 |
| 1 | 0.060927 | 2.515441 | 0.318766 |
| 1 | -0.060927 | -2.515441 | 0.318766 |
| 15 | -1.579764 | 0.751947 | -0.588385 |
| 15 | 1.579764 | -0.751947 | -0.588385 |
| 7 | -1.138513 | -0.796068 | -0.150166 |
| 7 | 1.138513 | 0.796068 | -0.150166 |

**16P-π**

| | | | |
|---|---|---|---|
| 12 | -0.631699 | -0.134088 | 1.542327 |
| 7 | -0.713496 | -1.333551 | -0.355599 |
| 15 | 0.968015 | -1.263688 | -0.258358 |

| | | | |
|---|---|---|---|
| 15 | 1.467292 | 0.870775 | -0.107112 |
| 6 | -0.161687 | 1.580744 | -0.180750 |
| 6 | -1.382277 | 1.009231 | -0.600178 |
| 6 | -1.612271 | -0.380452 | -0.690697 |
| 1 | -0.183153 | 2.652390 | 0.014744 |
| 1 | -2.226491 | 1.669268 | -0.779616 |
| 1 | -2.607698 | -0.741184 | -0.942062 |

**17P-π**

| | | | |
|---|---|---|---|
| 12 | -0.787903 | -0.101997 | 1.489809 |
| 7 | -1.516150 | -0.738477 | -0.615135 |
| 6 | -0.395407 | -1.467654 | -0.396442 |
| 15 | 1.321602 | -1.029943 | -0.170203 |
| 15 | 1.230623 | 1.133904 | -0.029152 |
| 6 | -0.475804 | 1.484627 | -0.372619 |
| 6 | -1.530011 | 0.615947 | -0.709019 |
| 1 | -0.592535 | -2.540053 | -0.355578 |
| 1 | -0.723134 | 2.545896 | -0.360263 |
| 1 | -2.492479 | 1.030519 | -0.997124 |

**19P-π**

| | | | |
|---|---|---|---|
| 12 | 0.172822 | 0.509329 | 1.552753 |
| 7 | 1.240836 | 0.913519 | -0.450381 |
| 15 | 1.558070 | -0.733633 | -0.357426 |
| 6 | -0.046590 | -1.391622 | 0.021544 |
| 15 | -1.664063 | -0.693478 | -0.177869 |
| 6 | -1.219267 | 0.992775 | -0.499653 |
| 6 | 0.065752 | 1.570858 | -0.584968 |
| 1 | -0.058512 | -2.449220 | 0.295928 |
| 1 | -2.060112 | 1.669793 | -0.637563 |
| 1 | 0.149430 | 2.647448 | -0.730852 |

**20P-π**

| | | | |
|---|---|---|---|
| 12 | -1.613641 | 0.415396 | 0.000000 |
| 7 | 0.273358 | 1.645637 | 0.000000 |
| 6 | 0.387137 | 1.014407 | 1.198186 |
| 15 | 0.387137 | -0.715452 | 1.618597 |
| 6 | 0.084121 | -1.364986 | 0.000000 |
| 15 | 0.387137 | -0.715452 | -1.618597 |
| 6 | 0.387137 | 1.014407 | -1.198186 |
| 1 | 0.410711 | 1.705420 | 2.040292 |
| 1 | -0.135709 | -2.434453 | 0.000000 |
| 1 | 0.410711 | 1.705420 | -2.040292 |

**24P-π**

| | | | |
|---|---|---|---|
| 12 | -0.229256 | 0.089582 | 1.657482 |
| 7 | -0.684374 | -1.269387 | -0.026223 |
| 15 | 0.973938 | -1.418557 | -0.222387 |
| 15 | 1.780100 | 0.626111 | -0.361099 |
| 6 | 0.322379 | 1.624554 | -0.122683 |
| 6 | -1.041695 | 1.357100 | -0.385722 |
| 15 | -1.887397 | -0.205157 | -0.507824 |
| 1 | 0.561048 | 2.659669 | 0.126826 |
| 1 | -1.703073 | 2.225167 | -0.412980 |

**25P-π**

| | | | |
|---|---|---|---|
| 12 | 0.146699 | -0.473803 | 1.623839 |
| 7 | -0.200822 | -1.573774 | -0.244151 |
| 15 | -1.639733 | -0.714254 | -0.417888 |
| 15 | -1.148620 | 1.412935 | -0.165588 |
| 6 | 0.592736 | 1.366896 | 0.155134 |
| 15 | 1.916236 | 0.344440 | -0.448187 |
| 6 | 1.077819 | -1.227754 | -0.524911 |
| 1 | 0.958980 | 2.301466 | 0.588278 |
| 1 | 1.744823 | -2.081083 | -0.671683 |

**26P-π**

| | | | |
|---|---|---|---|
| 12 | 0.280712 | -0.225512 | 1.671552 |
| 7 | 0.963790 | -1.296204 | -0.284316 |
| 15 | 1.869602 | 0.066700 | -0.629992 |
| 6 | 0.780734 | 1.321463 | -0.005159 |
| 15 | -0.994437 | 1.422674 | -0.114035 |
| 15 | -1.776056 | -0.573186 | -0.442948 |
| 6 | -0.332212 | -1.591382 | -0.121299 |
| 1 | 1.243248 | 2.269736 | 0.281663 |
| 1 | -0.536095 | -2.613471 | 0.213288 |

**27P-π**

| | | | |
|---|---|---|---|
| 12 | -1.625394 | 0.051795 | 0.000000 |
| 7 | 0.054399 | -1.517357 | 0.000000 |
| 15 | 0.290987 | -1.000928 | 1.566304 |
| 6 | 0.290987 | 0.769065 | 1.382727 |
| 15 | 0.417728 | 1.879035 | 0.000000 |
| 6 | 0.290987 | 0.769065 | -1.382727 |
| 15 | 0.290987 | -1.000928 | -1.566304 |
| 1 | 0.318286 | 1.306751 | 2.334552 |
| 1 | 0.318286 | 1.306751 | -2.334552 |

**39P-π**

| | | | |
|---|---|---|---|
| 7 | 0.707687 | 1.425375 | 0.337274 |
| 15 | 2.013050 | 0.765157 | -0.269226 |
| 15 | 1.218233 | -1.299924 | 0.139161 |
| 15 | -0.714394 | -1.204146 | -0.812196 |
| 15 | -1.670283 | 0.750629 | -0.749977 |
| 6 | -0.600496 | 1.554183 | 0.465879 |
| 1 | -0.993472 | 2.310529 | 1.151424 |
| 12 | -1.088037 | -0.565750 | 1.589663 |

**40P-π**

| | | | |
|---|---|---|---|
| 7 | -0.832169 | -1.077749 | -0.613759 |
| 15 | -1.624955 | 0.290512 | -1.105590 |
| 6 | -0.916696 | 1.357322 | 0.155167 |
| 15 | 0.861969 | 1.480058 | 0.358193 |
| 15 | 2.101533 | -0.031097 | -0.339174 |
| 15 | 0.575938 | -1.578250 | 0.089846 |
| 1 | -1.444326 | 2.288466 | 0.380850 |
| 12 | -1.328966 | -0.442209 | 1.494611 |

**41P-π**

| | | | |
|---|---|---|---|
| 7 | 0.097417 | -1.545992 | 0.000000 |
| 15 | -0.387900 | -1.082010 | 1.539294 |
| 15 | -0.387900 | 1.107460 | 1.602252 |
| 6 | 0.192274 | 1.595778 | 0.000000 |
| 15 | -0.387900 | 1.107460 | -1.602252 |
| 15 | -0.387900 | -1.082010 | -1.539294 |
| 1 | 0.743894 | 2.541354 | 0.000000 |
| 12 | 1.724547 | -0.171466 | 0.000000 |

Table S18: MP2/cc-pVTZ optimized geometries for the N-analogues $Mg^{2+}$-complexed cation-σ systems

**1N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 0.653627 |
| 6 | 0.000000 | 1.175125 | -0.037727 |
| 6 | 0.000000 | 1.201437 | -1.421957 |
| 6 | 0.000000 | 0.000000 | -2.127860 |
| 6 | 0.000000 | -1.201437 | -1.421957 |
| 6 | 0.000000 | -1.175125 | -0.037727 |
| 1 | 0.000000 | 2.095830 | 0.532254 |
| 1 | 0.000000 | 2.155567 | -1.929644 |
| 1 | 0.000000 | 0.000000 | -3.209490 |
| 1 | 0.000000 | -2.155567 | -1.929644 |
| 1 | 0.000000 | -2.095830 | 0.532254 |
| 12 | 0.000000 | 0.000000 | 2.642687 |

**2N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.364438 | -0.625792 |
| 6 | 0.000000 | 0.695532 | -1.851336 |
| 6 | 0.000000 | -0.695532 | -1.851336 |
| 6 | 0.000000 | -1.364438 | -0.625792 |
| 1 | 0.000000 | 2.442710 | -0.538713 |
| 1 | 0.000000 | 1.260625 | -2.773584 |
| 1 | 0.000000 | -1.260625 | -2.773584 |
| 1 | 0.000000 | -2.442710 | -0.538713 |
| 7 | 0.000000 | 0.681808 | 0.521090 |
| 7 | 0.000000 | -0.681808 | 0.521090 |
| 12 | 0.000000 | 0.000000 | 2.421240 |

**3N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.059269 | -2.085695 | 0.000000 |
| 6 | -1.121501 | -0.143241 | 0.000000 |
| 6 | 1.204365 | -0.002034 | 0.000000 |
| 6 | 1.264665 | -1.383124 | 0.000000 |
| 1 | 0.030980 | -3.167997 | 0.000000 |
| 1 | -2.085858 | 0.356366 | 0.000000 |
| 1 | 2.103627 | 0.599759 | 0.000000 |
| 1 | 2.220444 | -1.887334 | 0.000000 |
| 7 | 0.000000 | 0.636675 | 0.000000 |
| 7 | -1.124184 | -1.455736 | 0.000000 |
| 12 | -0.236724 | 2.626433 | 0.000000 |

**4N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.166041 | -0.060320 |
| 6 | 0.000000 | -1.166041 | -0.060320 |
| 6 | 0.000000 | -1.140269 | -1.453250 |
| 6 | 0.000000 | 1.140269 | -1.453250 |
| 1 | 0.000000 | 2.102392 | 0.482824 |
| 1 | 0.000000 | -2.102392 | 0.482824 |
| 1 | 0.000000 | -2.067884 | -2.011886 |
| 1 | 0.000000 | 2.067884 | -2.011886 |
| 7 | 0.000000 | 0.000000 | 0.640338 |
| 7 | 0.000000 | 0.000000 | -2.148870 |
| 12 | 0.000000 | 0.000000 | 2.648390 |

**5N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.299869 | 0.750074 | 0.000000 |
| 6 | -0.300498 | -1.502404 | 0.000000 |
| 6 | 1.083559 | -1.643696 | 0.000000 |
| 6 | 1.852930 | -0.477345 | 0.000000 |
| 1 | -0.995646 | -2.331912 | 0.000000 |
| 1 | 1.545167 | -2.622367 | 0.000000 |
| 1 | 2.935103 | -0.491713 | 0.000000 |
| 7 | 0.000000 | 0.811114 | 0.000000 |
| 7 | -0.823748 | -0.268359 | 0.000000 |
| 12 | -1.886118 | 1.511405 | 0.000000 |

**6N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.837883 | 0.000000 |
| 6 | -1.117093 | -1.602979 | 0.000000 |
| 6 | -1.325442 | 0.665957 | 0.000000 |
| 1 | -1.589900 | -2.577779 | 0.000000 |
| 1 | -1.940083 | 1.557377 | 0.000000 |
| 7 | 0.814665 | -0.253333 | 0.000000 |
| 6 | 0.283528 | -1.474864 | 0.000000 |
| 1 | 0.968401 | -2.312629 | 0.000000 |
| 7 | -1.910740 | -0.533065 | 0.000000 |
| 12 | 1.932346 | 1.453663 | 0.000000 |

**7N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.187766 | -1.426857 |
| 6 | 0.000000 | 0.000000 | -2.049133 |
| 1 | 0.000000 | 0.000000 | -3.131941 |
| 7 | 0.000000 | -1.187766 | -1.426857 |
| 7 | 0.000000 | 0.000000 | 0.618471 |
| 6 | 0.000000 | -1.153371 | -0.114649 |
| 1 | 0.000000 | -2.101538 | 0.413387 |
| 6 | 0.000000 | 1.153371 | -0.114649 |
| 1 | 0.000000 | 2.101538 | 0.413387 |
| 12 | 0.000000 | 0.000000 | 2.635204 |

**8N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 0.703557 | -1.775151 |
| 6 | 0.000000 | -0.703557 | -1.775151 |
| 1 | 0.000000 | 1.289276 | -2.686477 |
| 1 | 0.000000 | -1.289276 | -2.686477 |
| 7 | 0.000000 | 1.399567 | -0.627356 |
| 7 | 0.000000 | 0.675020 | 0.462490 |
| 7 | 0.000000 | -0.675020 | 0.462490 |
| 7 | 0.000000 | -1.399567 | -0.627356 |
| 12 | 0.000000 | 0.000000 | 2.415241 |

**9N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 6 | 0.212969 | -1.501503 | 0.000000 |
| 1 | 0.847489 | -2.380091 | 0.000000 |
| 1 | -2.905527 | -0.570631 | 0.000000 |
| 7 | -1.297884 | 0.742620 | 0.000000 |
| 7 | 0.000000 | 0.798036 | 0.000000 |
| 7 | 0.800809 | -0.292629 | 0.000000 |
| 7 | -1.110062 | -1.634851 | 0.000000 |
| 6 | -1.824219 | -0.507971 | 0.000000 |
| 12 | 1.914625 | 1.476278 | 0.000000 |

**10N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 1 | 0.000000 | 2.392300 | -0.697634 |
| 1 | 0.000000 | -2.392300 | -0.697634 |
| 7 | 0.000000 | -0.678534 | 0.485448 |
| 7 | 0.000000 | 0.678534 | 0.485448 |
| 7 | 0.000000 | -0.661027 | -1.872344 |
| 6 | 0.000000 | -1.309511 | -0.690206 |
| 7 | 0.000000 | 0.661027 | -1.872344 |
| 6 | 0.000000 | 1.309511 | -0.690206 |

| | | | |
|---|---|---|---|
| 12 | 0.000000 | 0.000000 | 2.424523 |

**11N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 1 | 0.780640 | -2.412022 | 0.000000 |
| 7 | 0.000000 | 0.770889 | 0.000000 |
| 7 | 0.799148 | -0.316951 | 0.000000 |
| 7 | -1.888716 | -0.503498 | 0.000000 |
| 7 | -1.153946 | -1.603463 | 0.000000 |
| 6 | 0.188863 | -1.503768 | 0.000000 |
| 7 | -1.305402 | 0.710107 | 0.000000 |
| 12 | 1.910716 | 1.502920 | 0.000000 |

**13–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | 1.348234 | 0.784849 | 0.000000 |
| 6 | -0.000799 | -1.851805 | 0.000000 |
| 6 | 2.022800 | -0.431145 | 0.000000 |
| 1 | 1.899937 | 1.716603 | 0.000000 |
| 1 | -0.441338 | -2.842767 | 0.000000 |
| 1 | 3.104505 | -0.403741 | 0.000000 |
| 7 | 0.000000 | 0.858972 | 0.000000 |
| 12 | -1.625699 | 2.029591 | 0.000000 |
| 15 | -1.037741 | -0.480401 | 0.000000 |
| 6 | 1.381423 | -1.679152 | 0.000000 |
| 1 | 2.001458 | -2.568469 | 0.000000 |

**14–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 1.294902 | 0.514031 | 0.000000 |
| 6 | 1.679164 | -0.821276 | 0.000000 |
| 1 | 2.054729 | 1.285496 | 0.000000 |
| 1 | 2.742300 | -1.027978 | 0.000000 |
| 7 | 0.000000 | 0.921759 | 0.000000 |
| 12 | -0.476168 | 2.858636 | 0.000000 |
| 6 | 0.770220 | -1.872100 | 0.000000 |
| 1 | 1.166256 | -2.882477 | 0.000000 |
| 6 | -1.033683 | 0.031880 | 0.000000 |
| 15 | -0.965577 | -1.714460 | 0.000000 |
| 1 | -2.029232 | 0.470710 | 0.000000 |

**15–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.187175 | -0.324029 |
| 6 | 0.000000 | -1.187175 | -0.324029 |
| 6 | 0.000000 | -1.312031 | 1.049432 |
| 6 | 0.000000 | 1.312031 | 1.049432 |
| 1 | 0.000000 | 2.084270 | -0.935269 |
| 1 | 0.000000 | -2.084270 | -0.935269 |
| 1 | 0.000000 | -2.323169 | 1.439894 |
| 1 | 0.000000 | 2.323169 | 1.439894 |
| 7 | 0.000000 | 0.000000 | -0.996803 |
| 15 | 0.000000 | 0.000000 | 2.203599 |
| 12 | 0.000000 | 0.000000 | -2.982538 |

**16N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 12 | -1.642892 | 1.985401 | 0.000000 |
| 7 | -1.116036 | 0.035724 | 0.000000 |
| 7 | 0.000000 | 0.824442 | 0.000000 |
| 15 | 1.618079 | 0.346740 | 0.000000 |
| 6 | 1.388100 | -1.384162 | 0.000000 |
| 6 | 0.148524 | -2.011250 | 0.000000 |
| 6 | -1.054342 | -1.297056 | 0.000000 |
| 1 | 2.282586 | -1.999937 | 0.000000 |
| 1 | 0.092488 | -3.093333 | 0.000000 |
| 1 | -2.012990 | -1.799008 | 0.000000 |

**17N–σ″$_{1N}$**

| | | | |
|---|---|---|---|
| 12 | -1.654162 | 2.180963 | 0.000000 |
| 7 | -1.117415 | 0.240223 | 0.000000 |
| 7 | 0.000000 | 1.018787 | 0.000000 |
| 6 | 1.240470 | 0.530545 | 0.000000 |
| 15 | 1.730414 | -1.161567 | 0.000000 |
| 6 | 0.114041 | -1.828082 | 0.000000 |
| 6 | -1.067089 | -1.097480 | 0.000000 |
| 1 | 2.005208 | 1.300645 | 0.000000 |
| 1 | 0.021912 | -2.909496 | 0.000000 |
| 1 | -2.036016 | -1.582160 | 0.000000 |

**18N–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.784796 | 0.000000 |
| 15 | -1.154230 | -0.488493 | 0.000000 |
| 7 | -0.302349 | -1.851044 | 0.000000 |
| 6 | 1.031461 | -1.900432 | 0.000000 |
| 6 | 1.852632 | -0.763090 | 0.000000 |
| 6 | 1.336368 | 0.526797 | 0.000000 |
| 1 | 1.479307 | -2.889202 | 0.000000 |
| 1 | 2.927681 | -0.881883 | 0.000000 |
| 1 | 2.022029 | 1.365889 | 0.000000 |
| 12 | -1.026824 | 2.501390 | 0.000000 |

**19N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.967355 | 0.000000 |
| 6 | -1.145693 | 0.213076 | 0.000000 |
| 7 | -1.229239 | -1.081541 | 0.000000 |
| 15 | 0.048345 | -2.144729 | 0.000000 |
| 6 | 1.391936 | -1.020709 | 0.000000 |
| 6 | 1.218437 | 0.348472 | 0.000000 |
| 1 | -2.081600 | 0.776878 | 0.000000 |
| 1 | 2.410501 | -1.392890 | 0.000000 |
| 1 | 2.086758 | 0.998215 | 0.000000 |
| 12 | -0.277020 | 2.945251 | 0.000000 |

**20N–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.619962 | -0.862895 | 0.000000 |
| 6 | 1.269150 | 0.404416 | 0.000000 |
| 7 | 0.000000 | 0.895063 | 0.000000 |
| 6 | -1.067610 | 0.049946 | 0.000000 |
| 15 | -1.040044 | -1.697503 | 0.000000 |
| 6 | 0.711713 | -1.839938 | 0.000000 |
| 1 | 2.079979 | 1.128135 | 0.000000 |
| 1 | -2.045152 | 0.523758 | 0.000000 |
| 1 | 1.131585 | -2.842491 | 0.000000 |
| 12 | -0.198750 | 2.895118 | 0.000000 |

**21N–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.835736 | 0.000000 |
| 15 | -1.046398 | -0.498374 | 0.000000 |
| 6 | 0.069999 | -1.846607 | 0.000000 |
| 7 | 1.384818 | -1.690979 | 0.000000 |
| 6 | 1.992740 | -0.491726 | 0.000000 |
| 6 | 1.347723 | 0.745225 | 0.000000 |
| 1 | -0.320821 | -2.860402 | 0.000000 |
| 1 | 3.076031 | -0.518516 | 0.000000 |
| 1 | 1.921832 | 1.663746 | 0.000000 |
| 12 | -1.594798 | 2.061344 | 0.000000 |

**22N–$\sigma''_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.039468 | -1.313549 | 0.000000 |
| 7 | -1.073341 | -0.016500 | 0.000000 |
| 7 | 0.000000 | 0.825452 | 0.000000 |
| 15 | 1.636538 | 0.392796 | 0.000000 |
| 6 | 1.402039 | -1.334895 | 0.000000 |
| 6 | 0.150812 | -1.948245 | 0.000000 |
| 1 | 2.283386 | -1.969915 | 0.000000 |
| 1 | 0.060999 | -3.028352 | 0.000000 |
| 12 | -1.784992 | 1.861445 | 0.000000 |

**23N–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | -1.065864 | -1.112202 | 0.000000 |
| 7 | -1.084604 | 0.191996 | 0.000000 |
| 7 | 0.000000 | 1.014059 | 0.000000 |
| 6 | 1.257759 | 0.564467 | 0.000000 |
| 15 | 1.752940 | -1.123424 | 0.000000 |
| 6 | 0.103563 | -1.763071 | 0.000000 |
| 1 | 2.009071 | 1.348441 | 0.000000 |
| 1 | -0.022270 | -2.842181 | 0.000000 |
| 12 | -1.782963 | 2.073312 | 0.000000 |

**24N–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | -1.095910 | 0.021316 | 0.000000 |
| 7 | 0.000000 | 0.839805 | 0.000000 |
| 15 | 1.606114 | 0.287961 | 0.000000 |
| 7 | 1.409871 | -1.341413 | 0.000000 |
| 6 | 0.248888 | -1.974004 | 0.000000 |
| 6 | -0.997871 | -1.308096 | 0.000000 |
| 1 | 0.263509 | -3.060461 | 0.000000 |
| 1 | -1.936099 | -1.848057 | 0.000000 |
| 12 | -1.676912 | 1.970313 | 0.000000 |

**25N–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.818954 | 0.000000 |
| 7 | -1.094448 | 0.004030 | 0.000000 |
| 6 | -0.982074 | -1.326145 | 0.000000 |
| 7 | 0.161776 | -2.014701 | 0.000000 |
| 6 | 1.338650 | -1.396419 | 0.000000 |
| 15 | 1.623650 | 0.351395 | 0.000000 |
| 1 | -1.912385 | -1.881086 | 0.000000 |
| 1 | 2.206345 | -2.052944 | 0.000000 |
| 12 | -1.688288 | 1.945042 | 0.000000 |

**26N–$\sigma''_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.016816 | 0.000000 |
| 7 | -1.088455 | 0.195607 | 0.000000 |
| 6 | -0.970289 | -1.141985 | 0.000000 |
| 7 | 0.167902 | -1.808820 | 0.000000 |
| 15 | 1.684225 | -1.162492 | 0.000000 |
| 6 | 1.255157 | 0.569932 | 0.000000 |
| 1 | -1.908801 | -1.687846 | 0.000000 |
| 1 | 2.004533 | 1.355920 | 0.000000 |
| 12 | -1.718704 | 2.114700 | 0.000000 |

**27N–$\sigma'_{1N}$**

| | | | |
|---|---|---|---|
| 15 | -1.255403 | -0.438601 | 0.000000 |
| 7 | 0.000000 | 0.746254 | 0.000000 |
| 7 | -0.474453 | -1.841167 | 0.000000 |
| 7 | 1.728012 | -0.919890 | 0.000000 |
| 6 | 1.304784 | 0.323903 | 0.000000 |
| 6 | 0.854571 | -1.940504 | 0.000000 |
| 1 | 2.084844 | 1.080547 | 0.000000 |
| 1 | 1.284255 | -2.936708 | 0.000000 |
| 12 | -0.522424 | 2.686533 | 0.000000 |

**28–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.248231 | 0.502301 | 0.000000 |
| 7 | 0.000000 | 1.049201 | 0.000000 |
| 15 | -1.538674 | 0.352599 | 0.000000 |
| 15 | -1.202997 | -1.770937 | 0.000000 |
| 6 | 0.548015 | -1.830951 | 0.000000 |
| 6 | 1.495615 | -0.814674 | 0.000000 |
| 1 | 0.956814 | -2.838815 | 0.000000 |
| 1 | 2.552494 | -1.054156 | 0.000000 |
| 12 | 1.384697 | 2.515108 | 0.000000 |

**29–$\sigma''_{2N}$**

| | | | |
|---|---|---|---|
| 7 | -1.152052 | 0.376188 | 0.000000 |
| 7 | 0.000000 | 1.108656 | 0.000000 |
| 15 | 1.613784 | 0.614240 | 0.000000 |
| 6 | 1.463914 | -1.113789 | 0.000000 |
| 15 | 0.074513 | -2.165017 | 0.000000 |
| 6 | -1.213340 | -0.955007 | 0.000000 |
| 1 | 2.422094 | -1.634997 | 0.000000 |
| 1 | -2.235196 | -1.322428 | 0.000000 |
| 12 | -1.579204 | 2.353162 | 0.000000 |

**30–$\sigma''_{3N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.684926 | 0.787099 |
| 15 | 0.000000 | -1.775083 | -0.499895 |
| 6 | 0.000000 | -0.693849 | -1.876889 |
| 6 | 0.000000 | 0.693849 | -1.876889 |
| 1 | 0.000000 | -1.197166 | -2.841724 |
| 1 | 0.000000 | 1.197166 | -2.841724 |
| 15 | 0.000000 | 1.775083 | -0.499895 |
| 7 | 0.000000 | -0.684926 | 0.787099 |
| 12 | 0.000000 | 0.000000 | 2.681966 |

**31–$\sigma''_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.680481 | 1.084433 |
| 7 | 0.000000 | -0.680481 | 1.084433 |
| 6 | 0.000000 | -1.455464 | -0.003519 |
| 15 | 0.000000 | -1.075787 | -1.715575 |
| 15 | 0.000000 | 1.075787 | -1.715575 |
| 6 | 0.000000 | 1.455464 | -0.003519 |
| 1 | 0.000000 | -2.512200 | 0.252509 |
| 1 | 0.000000 | 2.512200 | 0.252509 |
| 12 | 0.000000 | 0.000000 | 2.985201 |

**32–$\sigma'_{3bN}$**

| | | | |
|---|---|---|---|
| 7 | -1.211829 | -1.588111 | 0.000000 |
| 15 | -1.518094 | -0.020169 | 0.000000 |
| 7 | 0.000000 | 0.801647 | 0.000000 |
| 15 | 1.546125 | 0.069974 | 0.000000 |
| 6 | 1.208481 | -1.625401 | 0.000000 |
| 6 | -0.046974 | -2.238829 | 0.000000 |
| 1 | 2.092037 | -2.258072 | 0.000000 |
| 1 | -0.106689 | -3.324104 | 0.000000 |
| 12 | -0.074337 | 2.793812 | 0.000000 |

**33–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | -0.892842 | -1.579882 | 0.000000 |
| 15 | -1.358691 | -0.038384 | 0.000000 |
| 7 | 0.000000 | 0.981701 | 0.000000 |
| 6 | 1.284883 | 0.565710 | 0.000000 |
| 15 | 1.893763 | -1.088381 | 0.000000 |
| 6 | 0.366048 | -2.002554 | 0.000000 |
| 1 | 2.044924 | 1.343261 | 0.000000 |
| 1 | 0.482511 | -3.086429 | 0.000000 |
| 12 | -1.184101 | 2.621081 | 0.000000 |

**35–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.075995 | 0.000000 |
| 6 | 1.328923 | 0.773416 | 0.000000 |
| 7 | 1.837075 | -0.427784 | 0.000000 |
| 15 | 1.133508 | -1.924273 | 0.000000 |
| 6 | -0.602334 | -1.615469 | 0.000000 |
| 15 | -1.266056 | -0.047109 | 0.000000 |
| 1 | 2.014112 | 1.617296 | 0.000000 |
| 1 | -1.297991 | -2.452926 | 0.000000 |
| 12 | -1.328914 | 2.576768 | 0.000000 |

**36–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.515790 | -1.348071 | 0.000000 |
| 6 | 2.074805 | -0.138685 | 0.000000 |
| 6 | 1.352209 | 1.053123 | 0.000000 |
| 7 | 0.000000 | 1.111915 | 0.000000 |
| 15 | -1.136452 | -0.159403 | 0.000000 |
| 15 | 0.069889 | -2.031987 | 0.000000 |
| 1 | 3.160229 | -0.099048 | 0.000000 |
| 1 | 1.881916 | 1.998545 | 0.000000 |
| 12 | -1.684692 | 2.261485 | 0.000000 |

**37–σ′$_{3aN}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.178707 | -1.650975 |
| 6 | 0.000000 | -1.178707 | -1.650975 |
| 1 | 0.000000 | 2.045666 | -2.310057 |
| 1 | 0.000000 | -2.045666 | -2.310057 |
| 7 | 0.000000 | 0.000000 | -2.274856 |
| 7 | 0.000000 | 0.000000 | 0.768937 |
| 15 | 0.000000 | -1.553920 | 0.059350 |
| 15 | 0.000000 | 1.553920 | 0.059350 |
| 12 | 0.000000 | 0.000000 | 2.766062 |

**38–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 6 | -0.755248 | -1.677035 | 0.000000 |
| 6 | 1.302784 | 0.613650 | 0.000000 |
| 1 | -1.480690 | -2.490058 | 0.000000 |
| 1 | 2.022402 | 1.429519 | 0.000000 |
| 12 | -1.306425 | 2.530780 | 0.000000 |
| 7 | 0.000000 | 0.978672 | 0.000000 |
| 7 | 0.522582 | -1.959531 | 0.000000 |
| 15 | 1.912737 | -1.046790 | 0.000000 |
| 15 | -1.366596 | -0.024043 | 0.000000 |

**39N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.052589 | -1.171045 | 0.000000 |
| 7 | -1.082490 | 0.138168 | 0.000000 |
| 7 | 0.000000 | 0.964881 | 0.000000 |
| 7 | 1.240336 | 0.597564 | 0.000000 |
| 15 | 1.743751 | -1.012382 | 0.000000 |
| 6 | 0.137881 | -1.786761 | 0.000000 |
| 1 | 0.055709 | -2.871315 | 0.000000 |
| 12 | -1.731339 | 2.089219 | 0.000000 |

**40N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.417186 | -1.299343 | 0.000000 |
| 6 | -0.246704 | -1.910007 | 0.000000 |
| 7 | 0.982974 | -1.318140 | 0.000000 |
| 7 | 1.049095 | -0.022903 | 0.000000 |
| 7 | 0.000000 | 0.844963 | 0.000000 |
| 15 | -1.627902 | 0.324481 | 0.000000 |
| 1 | -0.215399 | -2.994946 | 0.000000 |
| 12 | 1.817498 | 1.846311 | 0.000000 |

**42N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 15 | 1.225656 | -1.737024 | 0.000000 |
| 15 | 1.560324 | 0.394459 | 0.000000 |
| 7 | 0.000000 | 1.037771 | 0.000000 |
| 7 | -1.229989 | 0.439751 | 0.000000 |
| 7 | -1.499089 | -0.833714 | 0.000000 |
| 6 | -0.542757 | -1.770688 | 0.000000 |
| 1 | -0.973449 | -2.770083 | 0.000000 |
| 12 | -1.538014 | 2.418836 | 0.000000 |

**43N–σ″$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | -1.204716 | -0.963455 | 0.000000 |
| 7 | -1.128878 | 0.318787 | 0.000000 |
| 7 | 0.000000 | 1.091545 | 0.000000 |
| 15 | 1.635242 | 0.632839 | 0.000000 |
| 6 | 1.489794 | -1.096049 | 0.000000 |
| 15 | 0.052516 | -2.094131 | 0.000000 |
| 1 | 2.439608 | -1.633424 | 0.000000 |
| 12 | -1.696632 | 2.250080 | 0.000000 |

**45N–σ″$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | 1.434214 | -1.088348 | 0.000000 |
| 15 | 1.597395 | 0.523027 | 0.000000 |
| 7 | 0.000000 | 1.106144 | 0.000000 |
| 7 | -1.156061 | 0.367492 | 0.000000 |
| 6 | -1.213161 | -0.964084 | 0.000000 |
| 15 | 0.167552 | -2.114074 | 0.000000 |
| 1 | -2.231298 | -1.343857 | 0.000000 |
| 12 | -1.575917 | 2.358087 | 0.000000 |

**47N–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.019155 | 0.000000 |
| 7 | -0.828954 | -1.541607 | 0.000000 |
| 15 | -1.360528 | -0.042198 | 0.000000 |
| 7 | 1.685898 | -0.687138 | 0.000000 |
| 15 | 0.746914 | -2.054376 | 0.000000 |
| 6 | 1.301236 | 0.555259 | 0.000000 |
| 1 | 2.084443 | 1.313294 | 0.000000 |
| 12 | -0.557188 | 2.939241 | 0.000000 |

Table S18: MP2/cc-pVTZ optimized geometries for the P-analogues $Mg^{2+}$-complexed cation-σ systems

**5P–σ′$_{3aP}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.266235 | -1.837224 |
| 6 | 0.000000 | 0.000000 | -2.427440 |
| 6 | 0.000000 | -1.266235 | -1.837224 |
| 1 | 0.000000 | 2.101483 | -2.536345 |
| 1 | 0.000000 | 0.000000 | -3.512839 |
| 1 | 0.000000 | -2.101483 | -2.536345 |
| 15 | 0.000000 | -1.856379 | -0.193280 |
| 15 | 0.000000 | 0.000000 | 0.799901 |
| 15 | 0.000000 | 1.856379 | -0.193280 |
| 12 | 0.000000 | 0.000000 | 3.249728 |

**8P–σ′$_{3bP}$**

| | | | |
|---|---|---|---|
| 6 | 1.684752 | -1.465244 | 0.000000 |
| 6 | 0.555278 | -2.279453 | 0.000000 |
| 1 | 2.636255 | -1.997509 | 0.000000 |
| 1 | 0.785795 | -3.345858 | 0.000000 |
| 15 | 1.976046 | 0.258557 | 0.000000 |
| 15 | 0.000000 | 0.991279 | 0.000000 |
| 15 | -1.807642 | -0.049877 | 0.000000 |
| 15 | -1.185217 | -2.106610 | 0.000000 |
| 12 | -0.134170 | 3.450943 | 0.000000 |

**9P–σ′$_{3aP}$**

| | | | |
|---|---|---|---|
| 6 | 0.000000 | 1.412514 | 1.549845 |
| 1 | 0.000000 | 2.318222 | 2.164382 |
| 15 | 0.000000 | -1.889865 | -0.123897 |
| 15 | 0.000000 | 0.000000 | -1.060085 |
| 15 | 0.000000 | 1.889865 | -0.123897 |
| 6 | 0.000000 | -1.412514 | 1.549845 |
| 15 | 0.000000 | 0.000000 | 2.586450 |
| 1 | 0.000000 | -2.318222 | 2.164382 |
| 12 | 0.000000 | 0.000000 | -3.508791 |

**10P–σ′$_{2aP}$**

| | | | |
|---|---|---|---|
| 15 | 0.000000 | 1.185908 | 0.000000 |
| 15 | -1.851342 | 0.193641 | 0.000000 |
| 6 | 1.523870 | 0.403654 | 0.000000 |
| 15 | 1.880106 | -1.310239 | 0.000000 |
| 1 | 2.401539 | 1.047569 | 0.000000 |
| 15 | 0.074565 | -2.482334 | 0.000000 |
| 6 | -1.355046 | -1.474685 | 0.000000 |
| 1 | -2.252498 | -2.101896 | 0.000000 |
| 12 | -0.225993 | 3.639655 | 0.000000 |

**16P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 15 | -1.995531 | 0.363413 | 0.000000 |
| 7 | 1.148058 | -0.182516 | 0.000000 |
| 15 | 0.000000 | 1.073505 | 0.000000 |
| 6 | 0.896842 | -1.501894 | 0.000000 |
| 6 | -0.386759 | -2.046459 | 0.000000 |
| 6 | -1.593441 | -1.338933 | 0.000000 |
| 1 | -2.490457 | -1.956284 | 0.000000 |
| 1 | -0.447595 | -3.128513 | 0.000000 |
| 1 | 1.754873 | -2.163418 | 0.000000 |
| 12 | 2.464990 | 1.357982 | 0.000000 |

**17P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 1.128771 | 0.404231 | 0.000000 |
| 6 | 0.000000 | 1.170247 | 0.000000 |
| 15 | -1.696514 | 0.770793 | 0.000000 |
| 15 | -1.703461 | -1.364952 | 0.000000 |
| 6 | -0.002910 | -1.763732 | 0.000000 |
| 6 | 1.118556 | -0.954430 | 0.000000 |
| 1 | 0.191546 | 2.245659 | 0.000000 |
| 1 | 0.209874 | -2.829578 | 0.000000 |
| 1 | 2.093338 | -1.430336 | 0.000000 |
| 12 | 2.825800 | 1.448709 | 0.000000 |

**19P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.123476 | 0.000000 |
| 15 | -1.243715 | -0.019607 | 0.000000 |
| 6 | -0.578327 | -1.589266 | 0.000000 |
| 15 | 1.124453 | -1.986244 | 0.000000 |
| 6 | 1.880356 | -0.397832 | 0.000000 |
| 6 | 1.328511 | 0.873584 | 0.000000 |
| 1 | -1.286785 | -2.415557 | 0.000000 |
| 1 | 2.965898 | -0.432171 | 0.000000 |
| 1 | 1.981436 | 1.739306 | 0.000000 |
| 12 | -1.471238 | 2.501078 | 0.000000 |

**20P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | 1.090531 |
| 6 | 0.000000 | 1.202105 | 0.454256 |
| 15 | 0.000000 | 1.589765 | -1.255469 |
| 6 | 0.000000 | 0.000000 | -1.949839 |
| 15 | 0.000000 | -1.589765 | -1.255469 |
| 6 | 0.000000 | -1.202105 | 0.454256 |
| 1 | 0.000000 | 2.069010 | 1.111471 |
| 1 | 0.000000 | 0.000000 | -3.039651 |
| 1 | 0.000000 | -2.069010 | 1.111471 |
| 12 | 0.000000 | 0.000000 | 3.091252 |

**21P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.991569 | 0.000000 |
| 15 | -1.370767 | 0.000954 | 0.000000 |
| 6 | -0.841639 | -1.642112 | 0.000000 |
| 6 | 0.497458 | -1.998433 | 0.000000 |
| 15 | 1.959734 | -1.012066 | 0.000000 |
| 6 | 1.293077 | 0.611523 | 0.000000 |
| 1 | -1.614725 | -2.405791 | 0.000000 |
| 1 | 0.702888 | -3.067074 | 0.000000 |
| 1 | 2.019634 | 1.420024 | 0.000000 |
| 12 | -1.302973 | 2.537724 | 0.000000 |

**22P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.356988 | 0.194880 | 0.000000 |
| 15 | 0.000000 | 1.221831 | 0.000000 |
| 15 | -1.913433 | 0.379059 | 0.000000 |
| 15 | -1.455927 | -1.716216 | 0.000000 |
| 6 | 0.281367 | -1.980152 | 0.000000 |
| 6 | 1.393865 | -1.148775 | 0.000000 |
| 1 | 0.512359 | -3.043752 | 0.000000 |
| 1 | 2.381286 | -1.598033 | 0.000000 |
| 12 | 2.341370 | 1.981756 | 0.000000 |

**23P–σ′$_{1N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 0.000000 | -1.340148 |
| 6 | 0.000000 | 1.213531 | -0.726413 |
| 15 | 0.000000 | 1.732132 | 0.944170 |
| 15 | 0.000000 | 0.000000 | 2.178189 |
| 15 | 0.000000 | -1.732132 | 0.944170 |
| 6 | 0.000000 | -1.213531 | -0.726413 |
| 1 | 0.000000 | 2.056016 | -1.418801 |
| 1 | 0.000000 | -2.056016 | -1.418801 |
| 12 | 0.000000 | 0.000000 | -3.338528 |

**24P–σ′$_{3bN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.100782 | 0.000000 |
| 15 | -1.265121 | -0.031292 | 0.000000 |
| 15 | -0.685050 | -2.068482 | 0.000000 |
| 6 | 1.055121 | -1.863096 | 0.000000 |
| 6 | 1.926511 | -0.773726 | 0.000000 |
| 15 | 1.680652 | 0.954149 | 0.000000 |
| 1 | 1.543344 | -2.838104 | 0.000000 |
| 1 | 2.986420 | -1.025440 | 0.000000 |
| 12 | -1.531397 | 2.430281 | 0.000000 |

**25P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.235896 | 0.000000 |
| 15 | -1.308464 | 0.150725 | 0.000000 |
| 15 | -0.800140 | -1.917255 | 0.000000 |
| 6 | 0.928957 | -1.752838 | 0.000000 |
| 15 | 2.195849 | -0.532903 | 0.000000 |
| 6 | 1.321964 | 0.989631 | 0.000000 |
| 1 | 1.381191 | -2.749338 | 0.000000 |
| 1 | 1.952867 | 1.875627 | 0.000000 |
| 12 | -1.512355 | 2.607764 | 0.000000 |

**26P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.246414 | 0.000000 |
| 15 | -1.426248 | 0.340034 | 0.000000 |
| 6 | -1.124228 | -1.345353 | 0.000000 |
| 15 | 0.387405 | -2.211373 | 0.000000 |
| 15 | 1.993626 | -0.757827 | 0.000000 |
| 6 | 1.285050 | 0.844334 | 0.000000 |
| 1 | -2.024295 | -1.961732 | 0.000000 |
| 1 | 2.015016 | 1.651884 | 0.000000 |
| 12 | -1.273117 | 2.835714 | 0.000000 |

**39P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 1.378895 | 0.437858 | 0.000000 |
| 15 | 0.000000 | 1.439400 | 0.000000 |
| 15 | -1.951879 | 0.642871 | 0.000000 |
| 15 | -1.669380 | -1.463112 | 0.000000 |
| 15 | 0.361147 | -2.208148 | 0.000000 |
| 6 | 1.523470 | -0.896608 | 0.000000 |
| 1 | 2.557983 | -1.236955 | 0.000000 |
| 12 | 2.295885 | 2.282202 | 0.000000 |

**40P–σ′$_{3bN}$**

| | | | |
|---|---|---|---|
| 15 | 1.006602 | -2.107782 | 0.000000 |
| 15 | -1.123277 | -1.796246 | 0.000000 |
| 7 | 0.000000 | 1.320405 | 0.000000 |
| 15 | -1.344247 | 0.281584 | 0.000000 |
| 15 | 1.673619 | 1.114242 | 0.000000 |
| 6 | 1.903048 | -0.606184 | 0.000000 |
| 1 | 2.973683 | -0.834003 | 0.000000 |
| 12 | -1.465201 | 2.737608 | 0.000000 |

**42P–σ′′$_{2N}$**

| | | | |
|---|---|---|---|
| 7 | -1.245234 | 0.735277 | 0.000000 |
| 7 | 0.000000 | 1.286929 | 0.000000 |
| 15 | 1.569894 | 0.654408 | 0.000000 |
| 15 | 1.488610 | -1.475215 | 0.000000 |
| 15 | -0.582427 | -2.047566 | 0.000000 |
| 6 | -1.535081 | -0.571535 | 0.000000 |
| 1 | -2.610645 | -0.734078 | 0.000000 |
| 12 | -1.383615 | 2.752787 | 0.000000 |

**44P–σ′′$_{3N}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.203879 | 0.000000 |
| 7 | -1.181928 | 0.517040 | 0.000000 |
| 15 | -1.535561 | -1.136813 | 0.000000 |
| 6 | 0.018096 | -1.913187 | 0.000000 |
| 15 | 1.698200 | -1.428293 | 0.000000 |
| 15 | 1.623490 | 0.726651 | 0.000000 |
| 1 | -0.089239 | -3.001312 | 0.000000 |
| 12 | -1.544815 | 2.500902 | 0.000000 |

**45P–σ′$_{2aN}$**

| | | | |
|---|---|---|---|
| 7 | 0.000000 | 1.231424 | 0.000000 |
| 15 | -1.397279 | 0.274514 | 0.000000 |
| 7 | -1.113367 | -1.289969 | 0.000000 |
| 15 | 0.282617 | -2.170361 | 0.000000 |
| 15 | 1.991296 | -0.785663 | 0.000000 |
| 6 | 1.291170 | 0.830556 | 0.000000 |
| 1 | 2.025559 | 1.634226 | 0.000000 |
| 12 | -1.260710 | 2.834575 | 0.000000 |

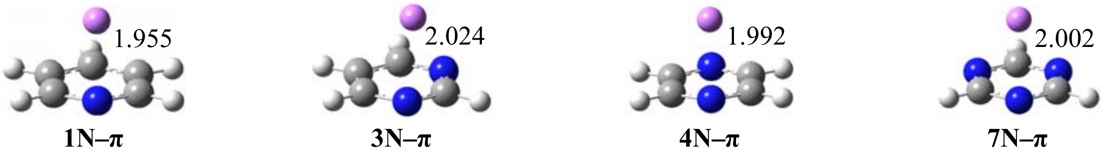



Figure S1a: Geometrical parameters of the homo-substituted N-analogs complexed with $Li^+$ in π–fashion.

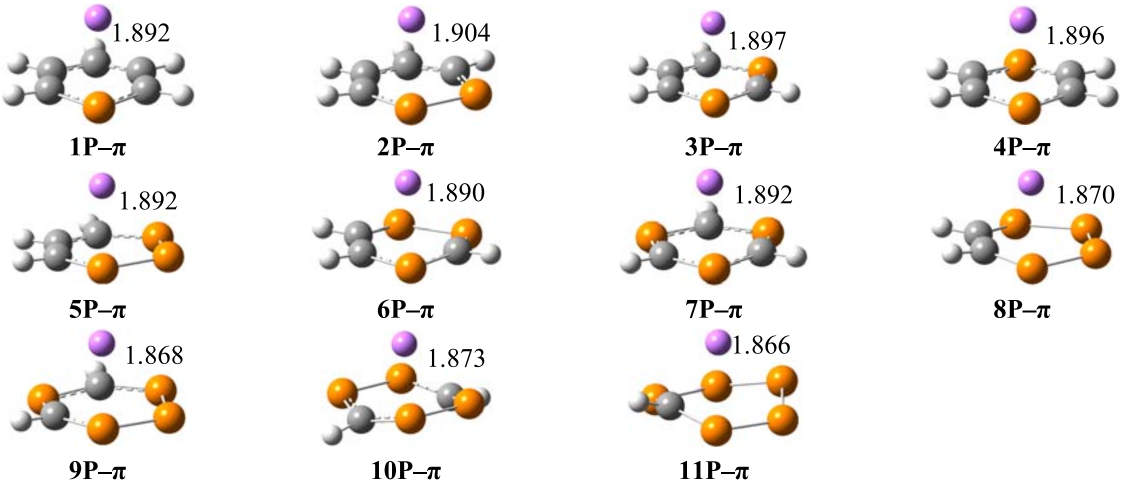



Figure S1b: Geometrical parameters of the homo-substituted P-analogs complexed with $Li^+$ in π–fashion.

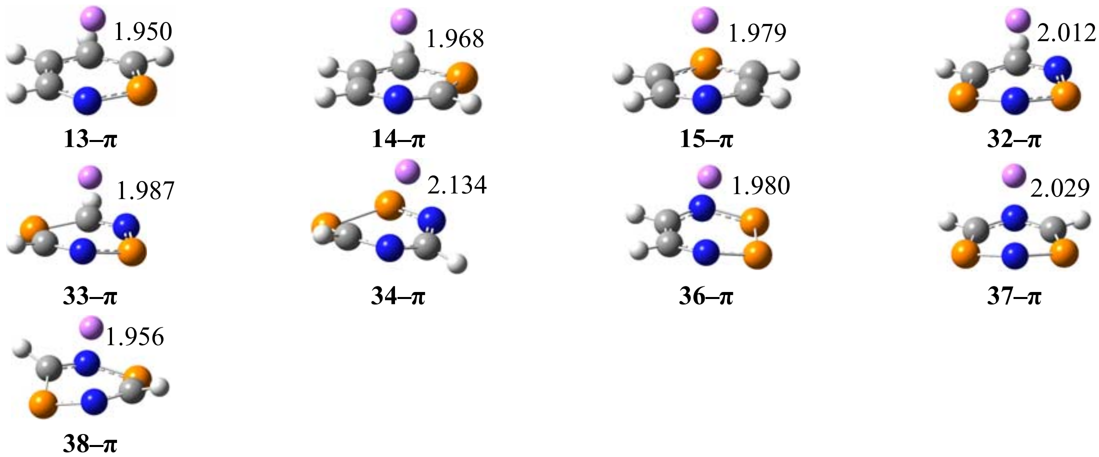



Figure S1c: Geometrical parameters of the P=N heteroaromatics complexed with $Li^+$ in π–fashion.


Figure S1d: Geometrical parameters of the hetero-substituted N-analogs complexed with $Li^+$ in π–fashion.

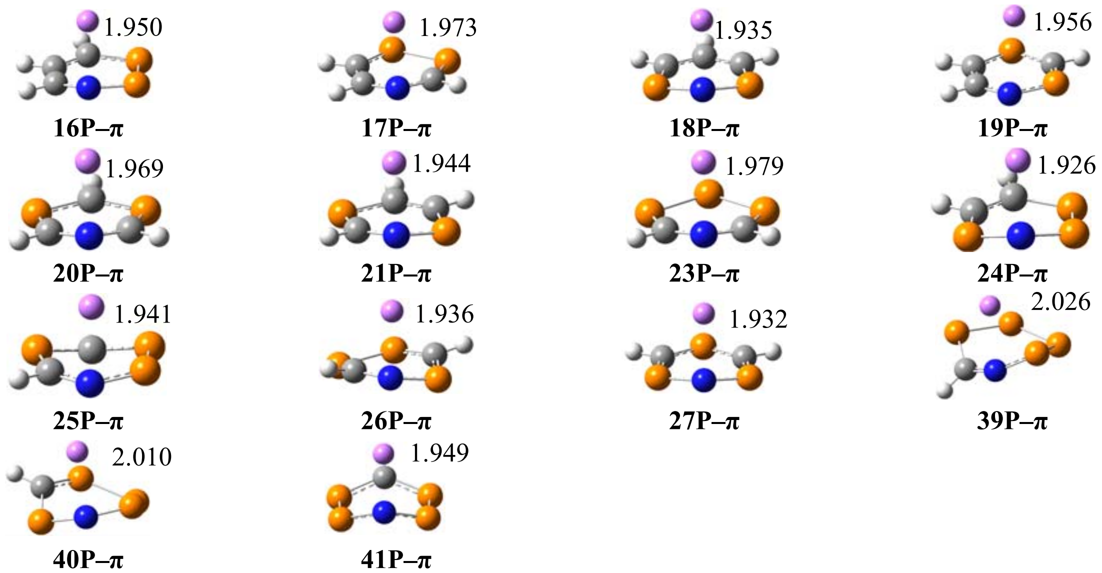



Figure S1e: Geometrical parameters of the hetero-substituted P-analogs complexed with $Li^+$ in π−fashion.

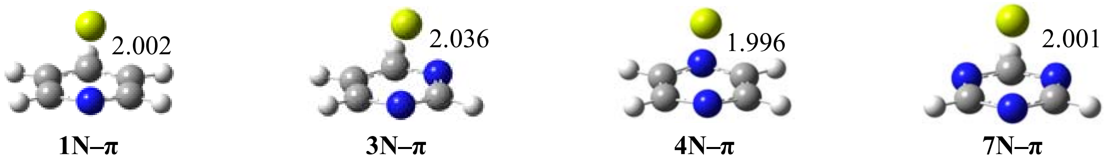



Figure S2a: Geometrical parameters of the homo-substituted N-analogs complexed with $Mg^{2+}$ in π–fashion.

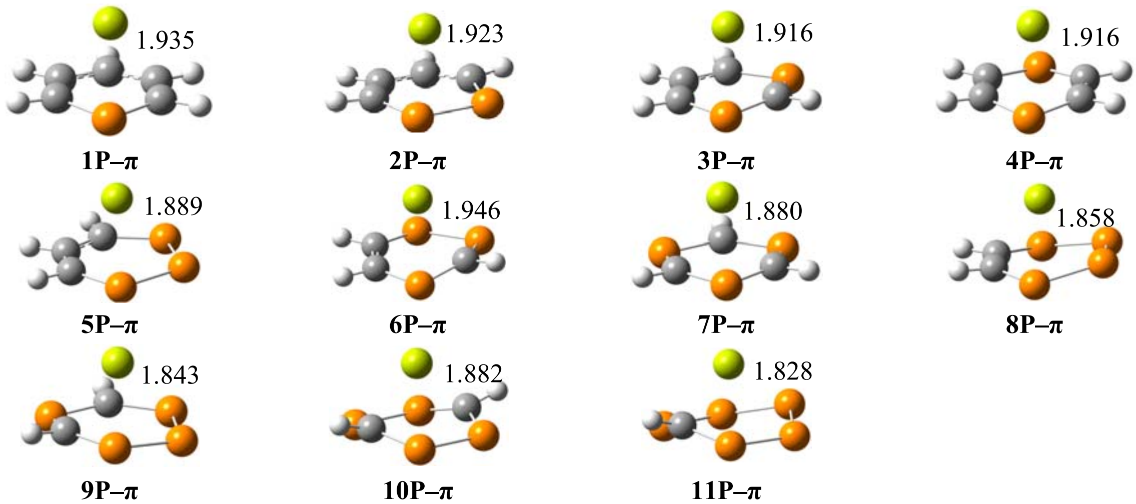



Figure S2b: Geometrical parameters of the homo-substituted N-analogs complexed with $Mg^{2+}$ in π–fashion.

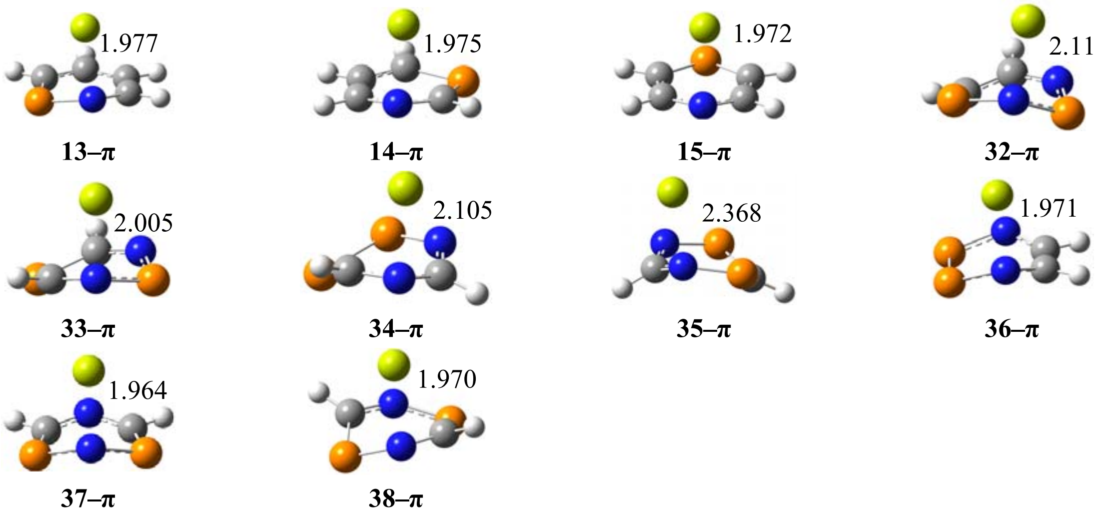


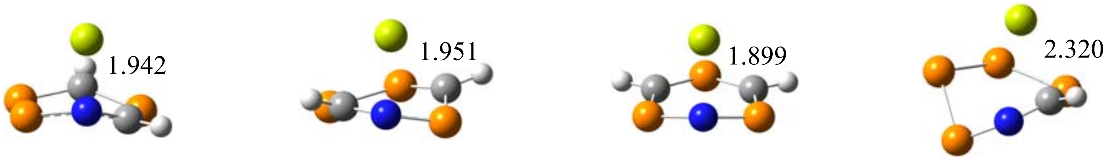

Figure S2c: Geometrical parameters of the heteroaromatics complex with $Mg^{2+}$ in π–fashion when there is equal number of P and N.


**18N–π** **19N–π** **20N–π** **21N–π**

Figure S2d: Geometrical parameters of the hetero-substituted N-analogs complexed with $Mg^{2+}$ in π–fashion.


**16P–π** **17P–π** **18P–π** **19P–π**


**20P–π** **21P–π** **23P–π** **24P–π**




**25P–π** **26P–π** **27P–π** **39P–π**


**40P–π** **41P–π**

Figure S2e: Geometrical parameters of the hetero-substituted P-analogs complexed with $Mg^{2+}$ in π–fashion.

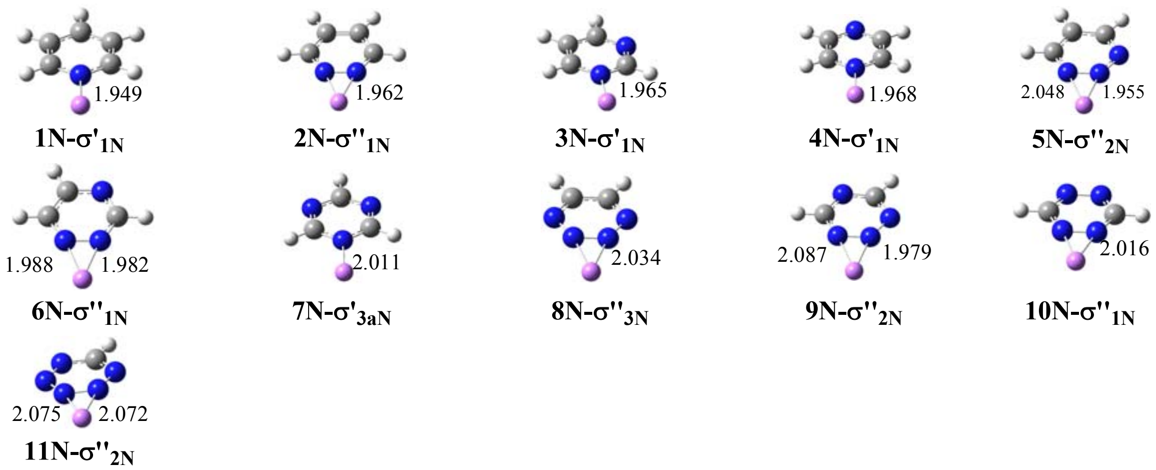



Figure S3a: Geometrical parameters of the homo-substituted N-analogs complexed with $Li^+$ in σ–fashion.

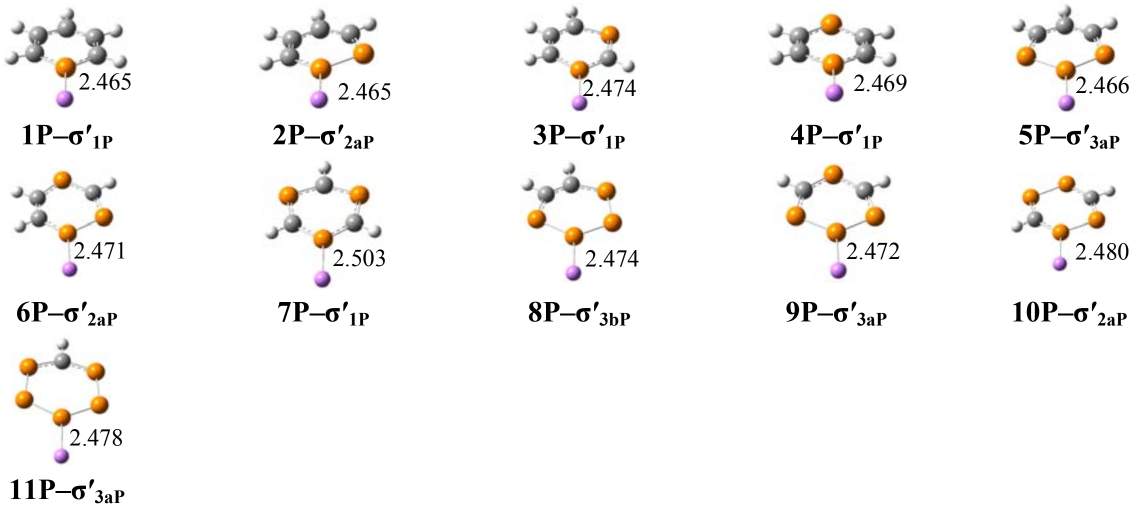



Figure S3b: Geometrical parameters of the homo-substituted P-analogs complexed with $Li^+$ in σ–fashion.

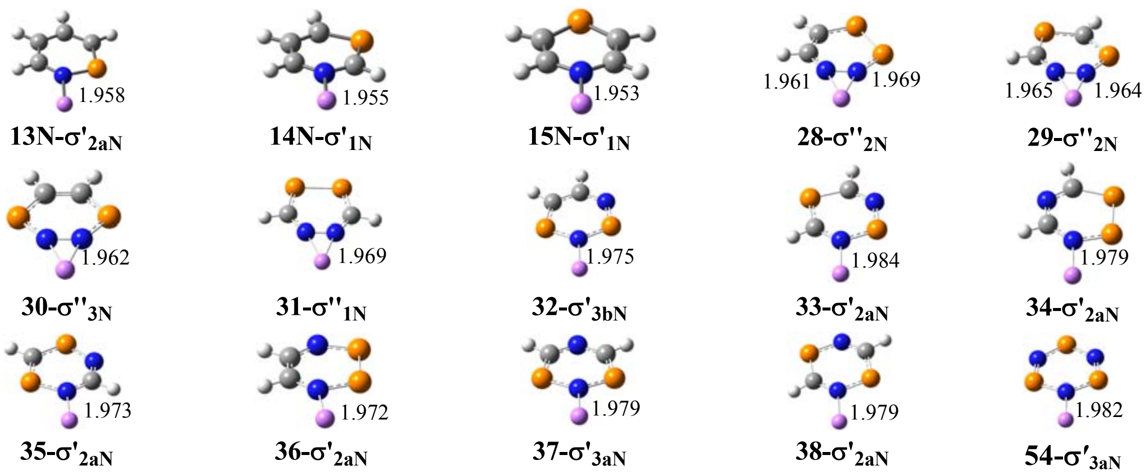



Figure S3c: Geometrical parameters of the heteroaromatics complexed with $Li^+$ in σ–fashion when there is equal number of P and N.

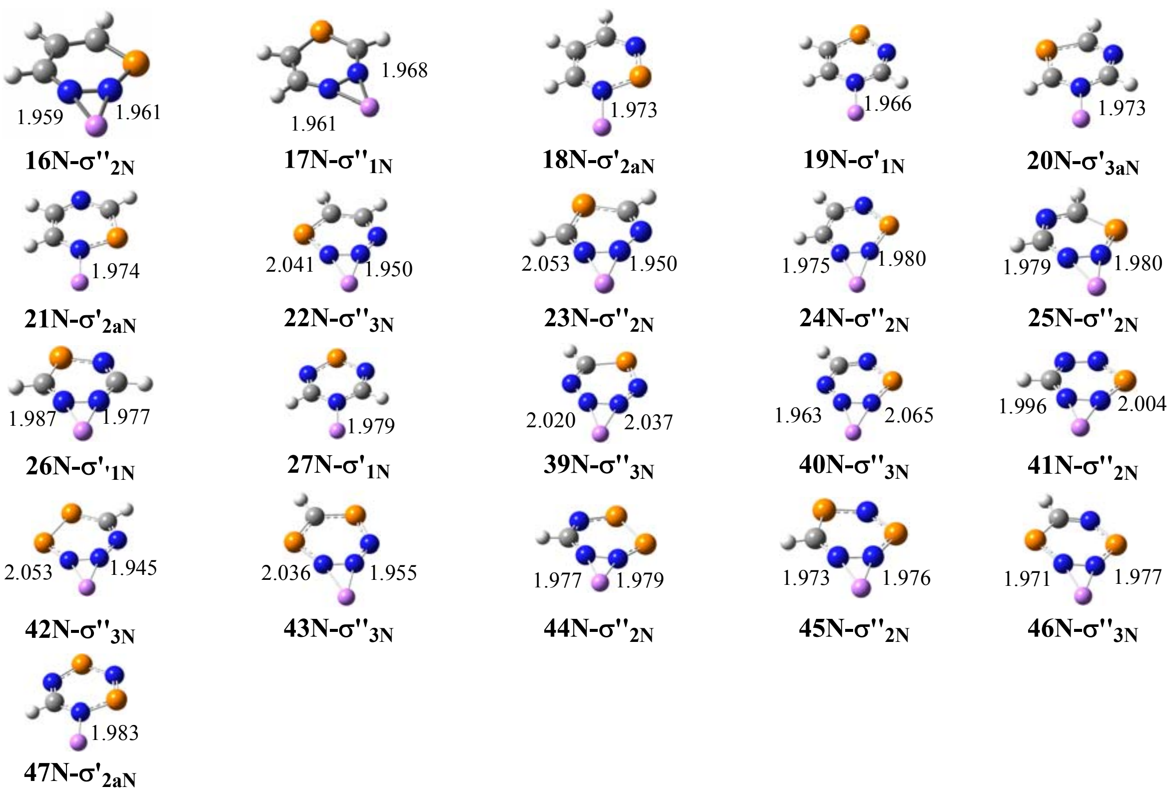



Figure S3d: Geometrical parameters of the hetero-substituted N-analogs complexed with $Li^+$ in σ–fashion.

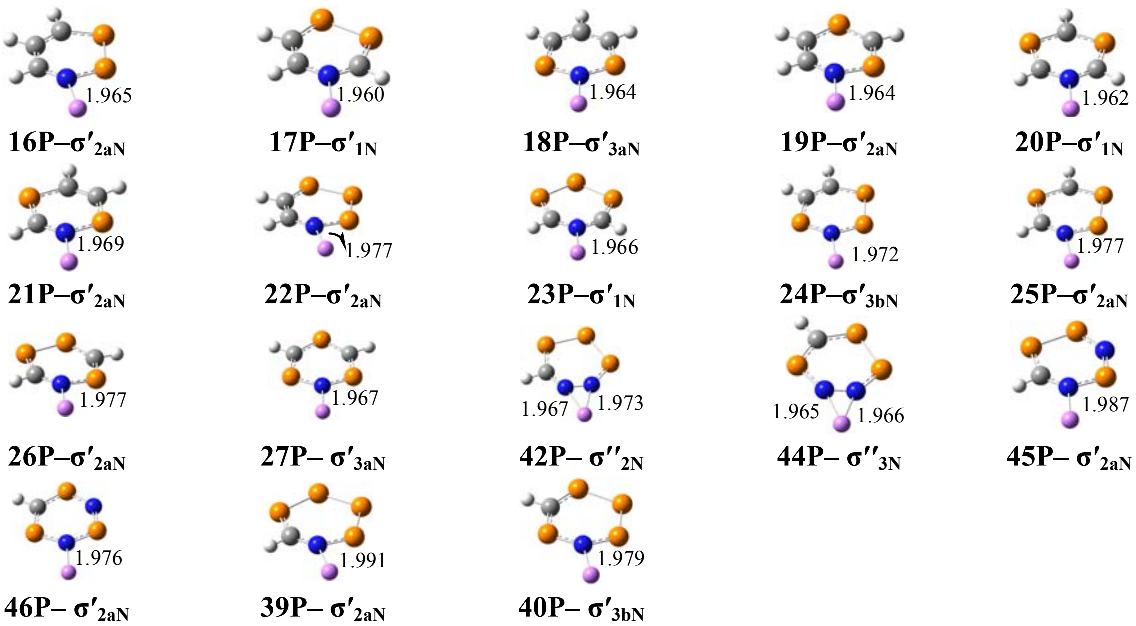



Figure S3e: Geometrical parameters of the hetero-substituted P-analogs complexed with $Li^+$ in σ–fashion.

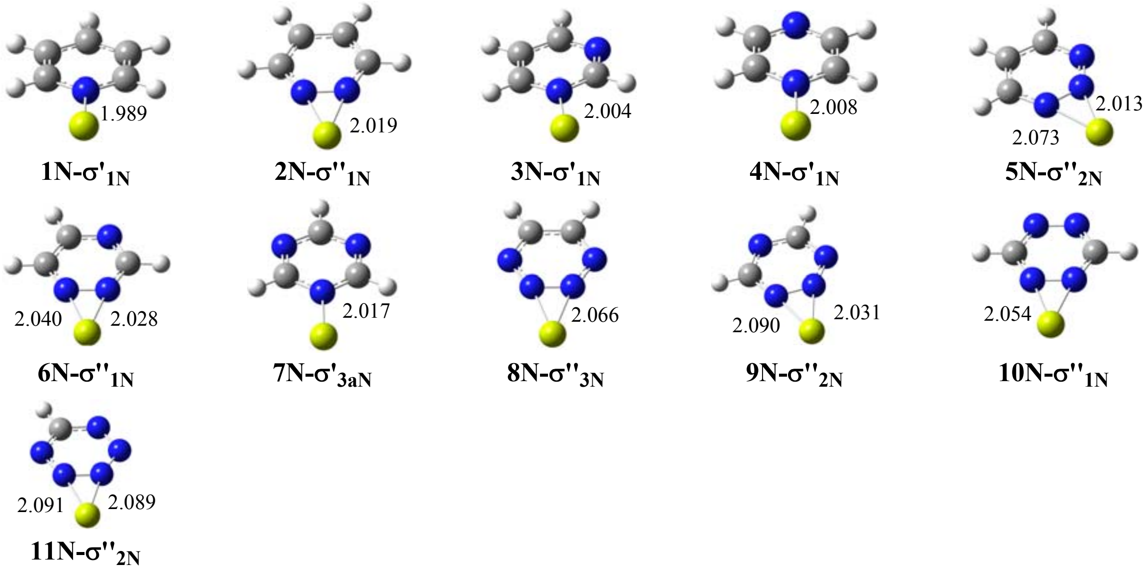



Figure S4a: Geometrical parameters of the homo-substituted N-analogs complexed with $Mg^{2+}$ in σ–fashion.

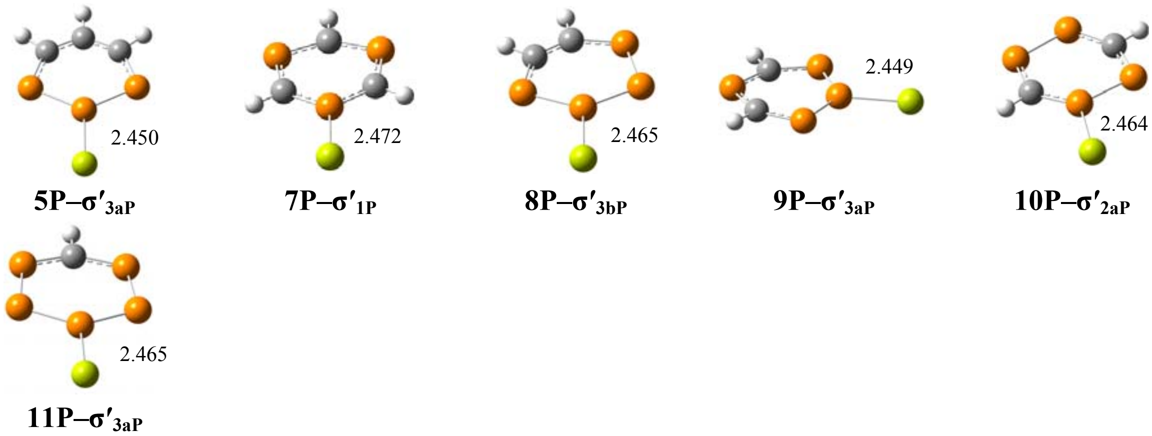



Figure S4b: Geometrical parameters of the homo-substituted N-analogs complexed with $Mg^{2+}$ in σ–fashion.

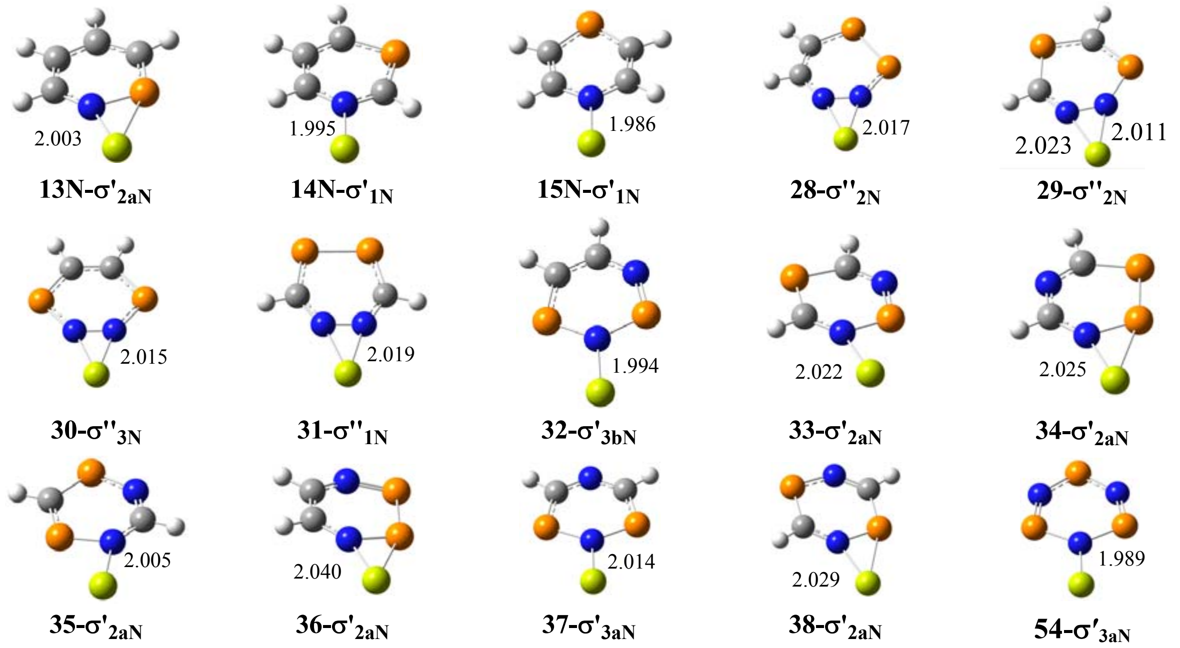



Figure S4c: Geometrical parameters of the heteroaromatics complexed with $Mg^{2+}$ in σ–fashion when number of P and N are equal.

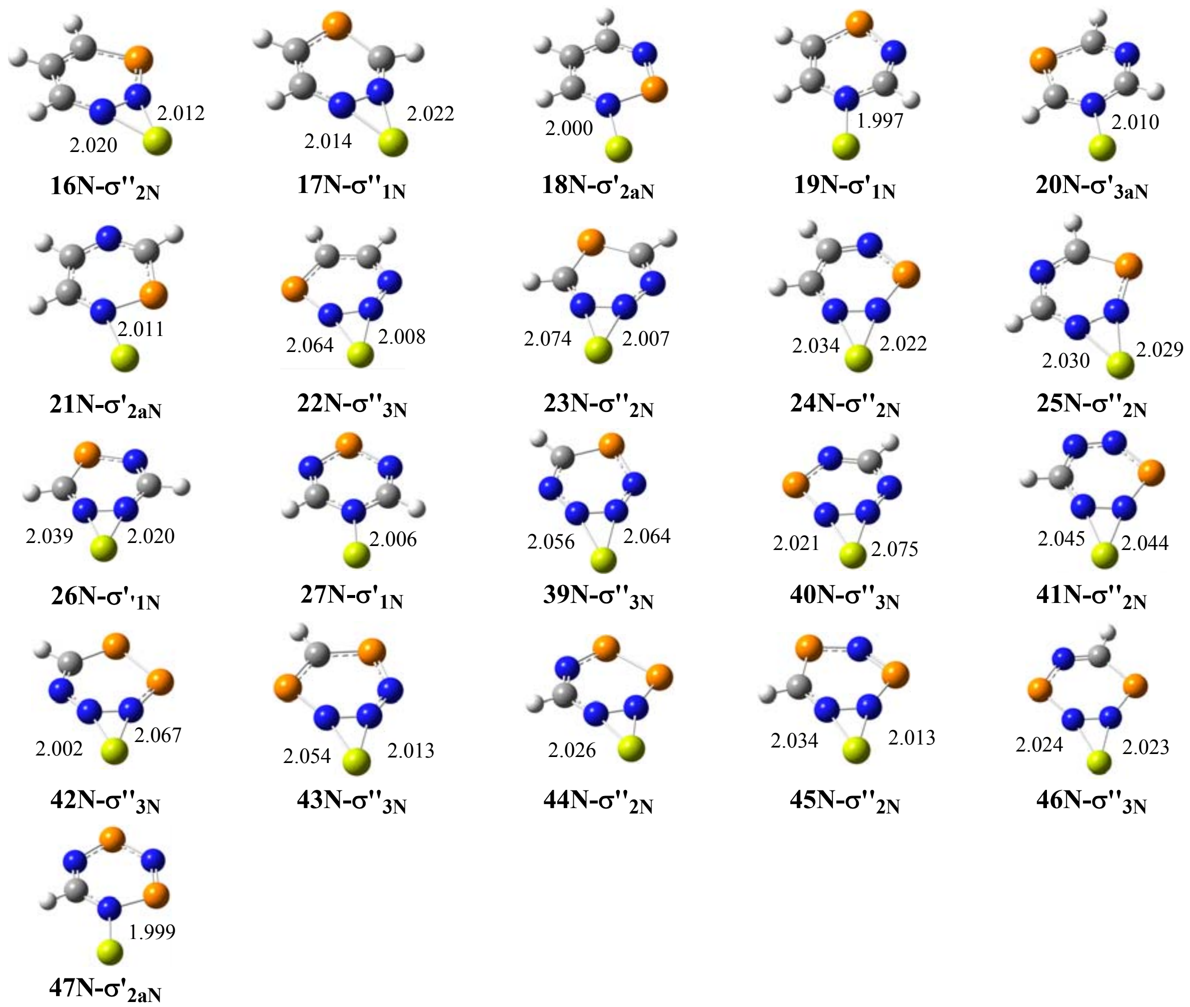



Figure S4d: Geometrical parameters of the hetero-substituted N-analogs complexed with $Mg^{2+}$ in σ–fashion

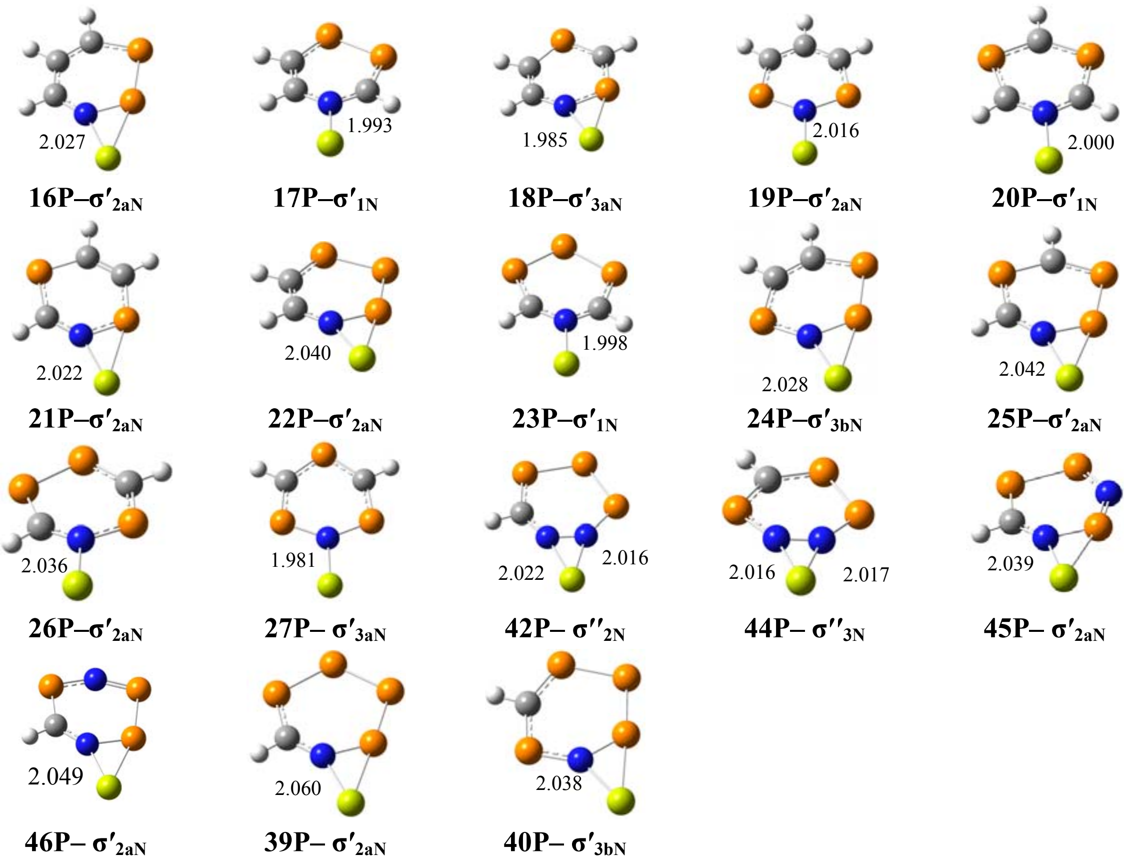



Figure S4e: Geometrical parameters of the hetero-substituted P-analogs complexed with $Mg^{2+}$ in σ–fashion

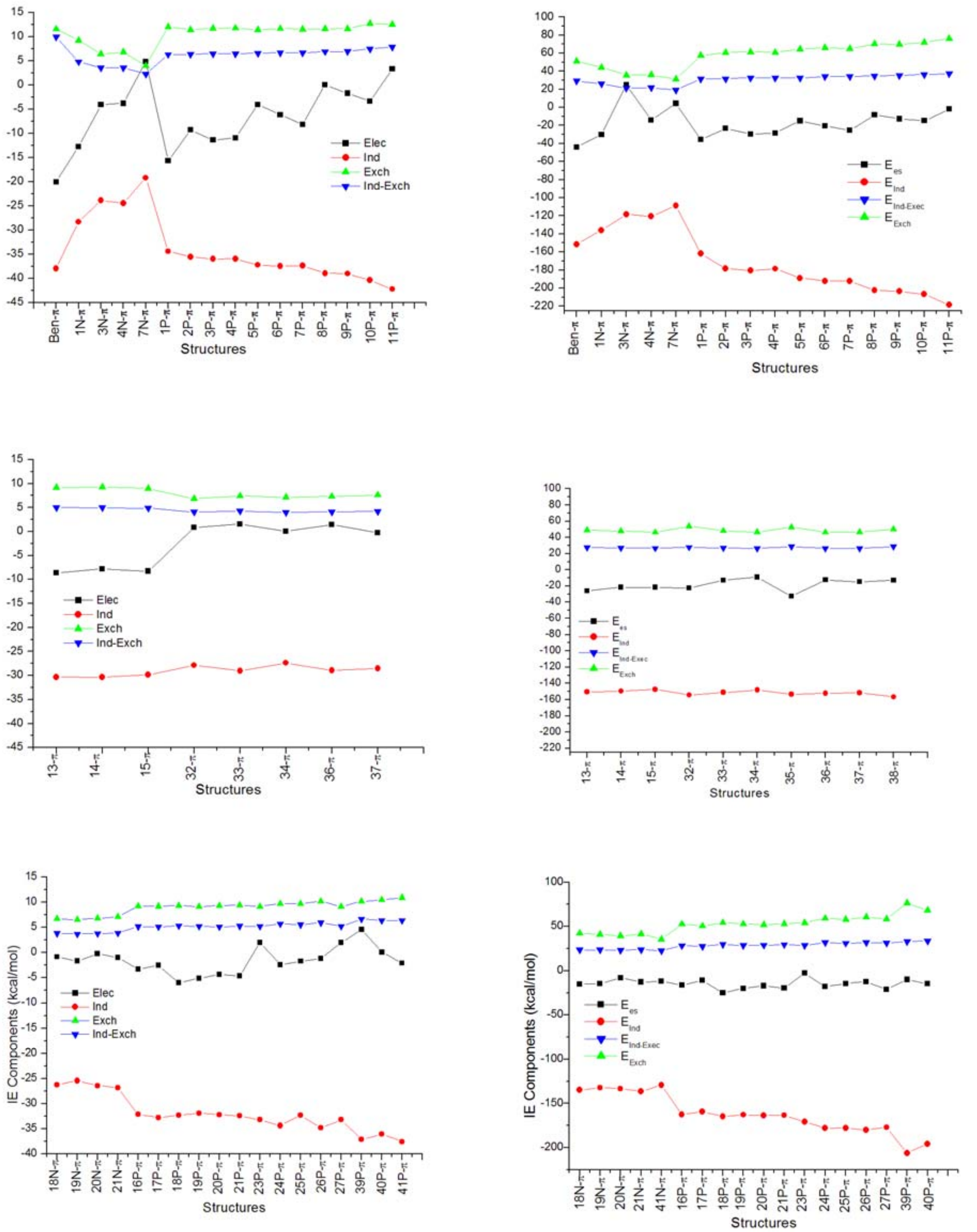



Fig. S5 Plots showing the variation in the components of the total interaction energy for the cation-π complexes obtained from HF-SAPT.

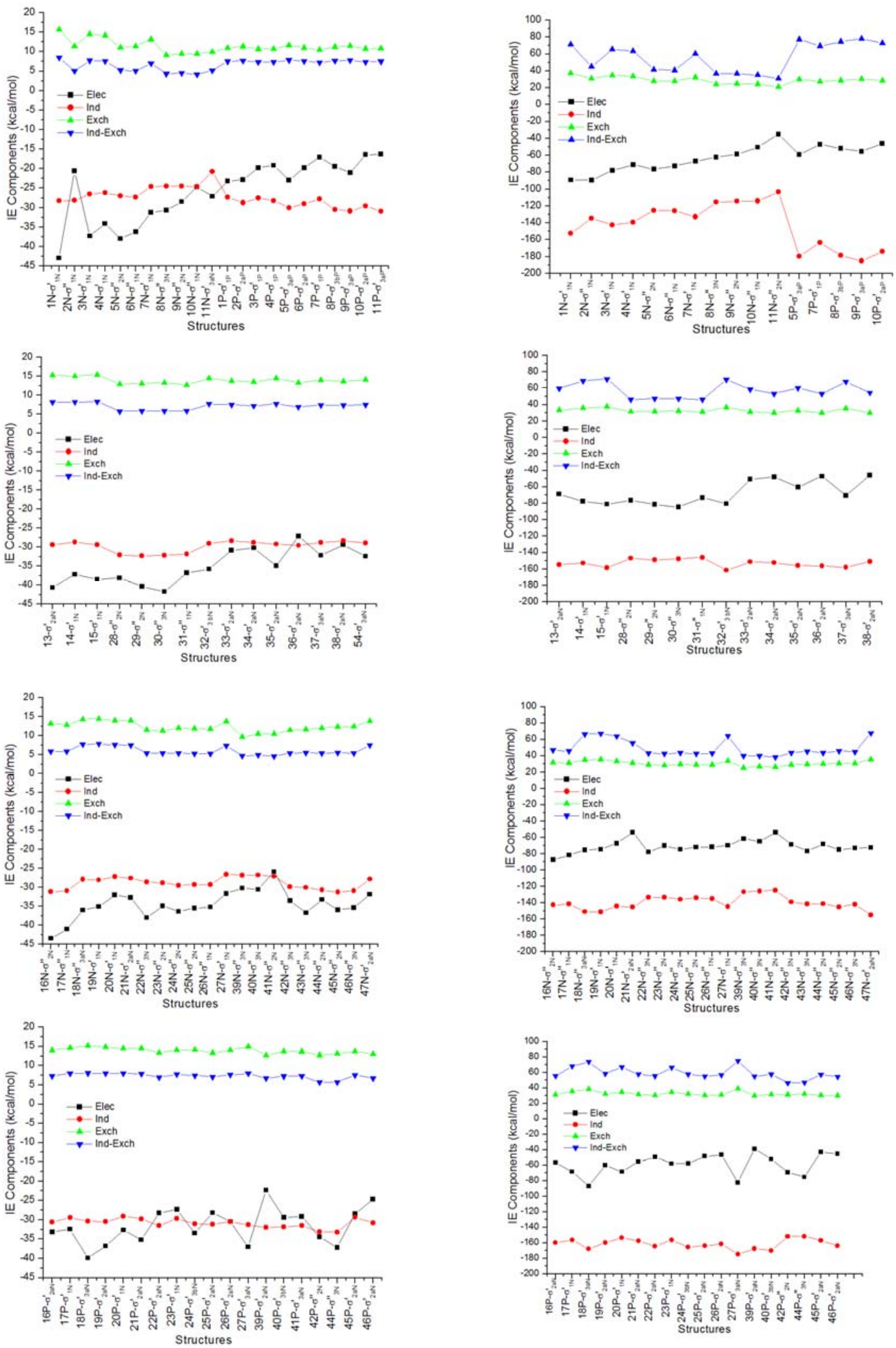



Fig. S6 Plots showing the variation in the components of the total interaction energy for the cation-σ complexes obtained from HF-SAPT.

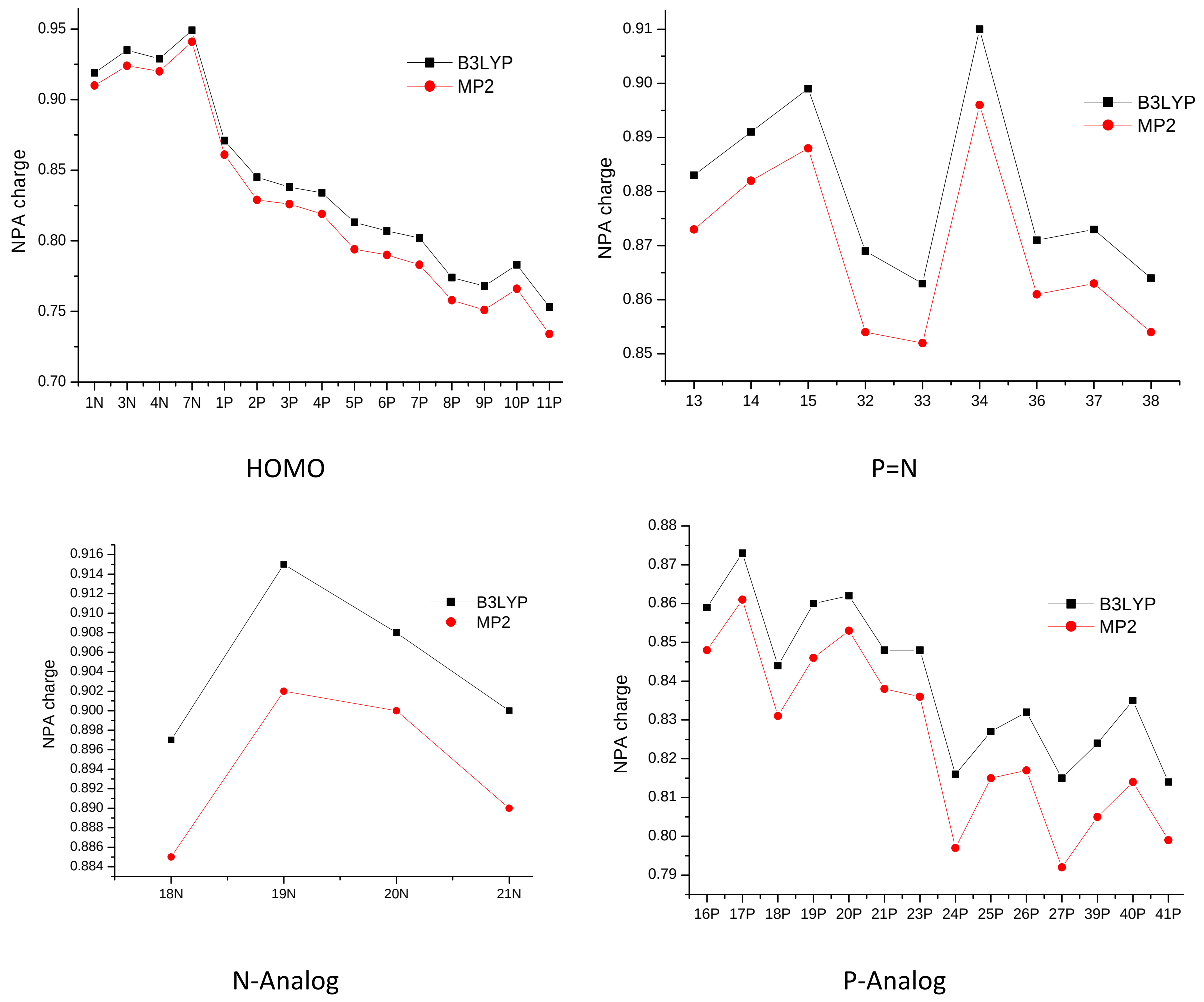



Fig. S7: Comparison between MP2 and B3LYP NPA charge with cc-pVTZ basis set for the $Li^+$-π complexes.

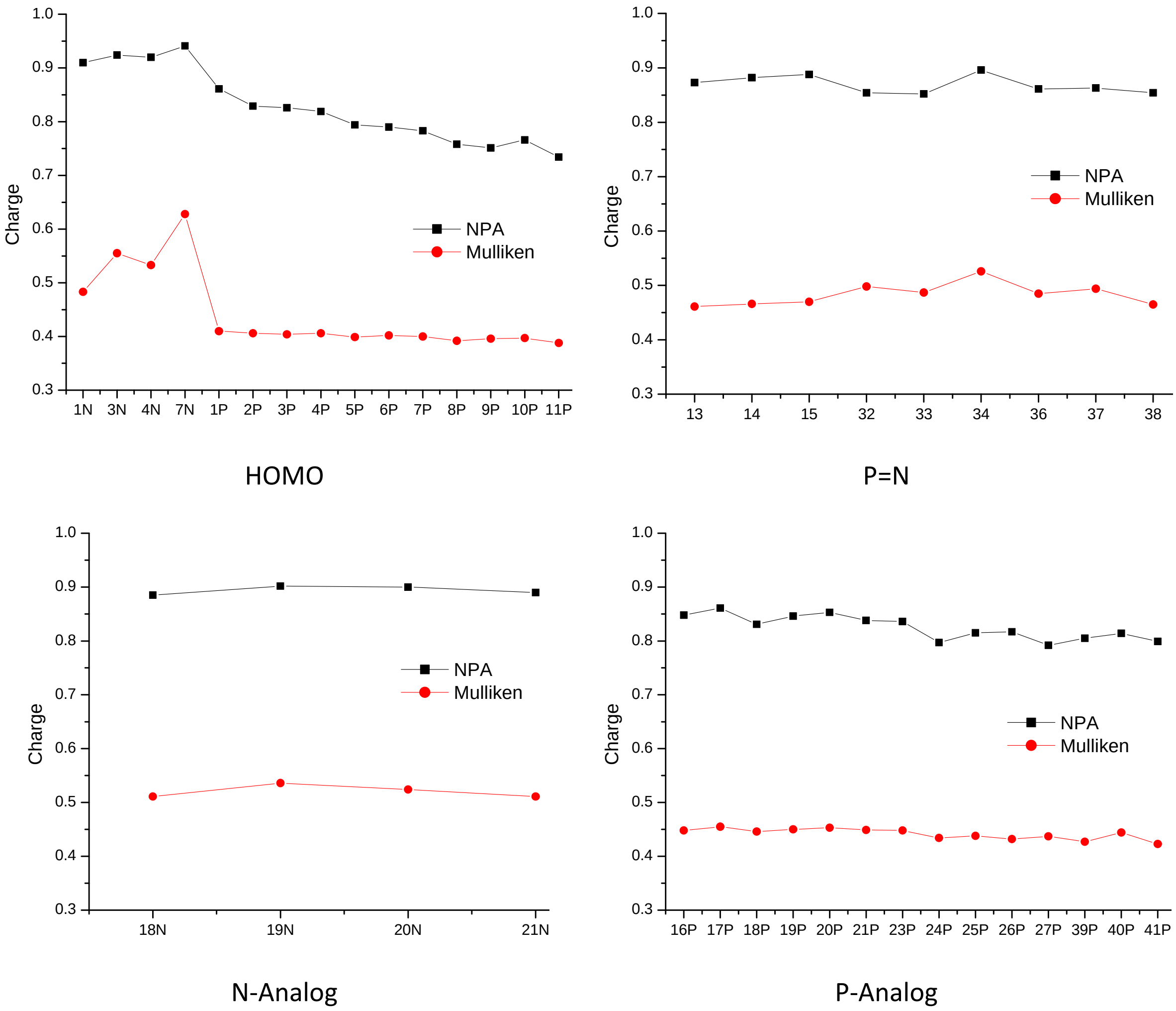



Fig S8: Comparison between NPA and Mulliken charge at MP2/cc-pVTZ level for the $Li^+$-$\pi$ complexes.