Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Supporting Information: Shedding Light on the Physical Nature of Ion Pair Interactions Involving Carba-*closo*-dodecaborate Anions. Insights from Computation

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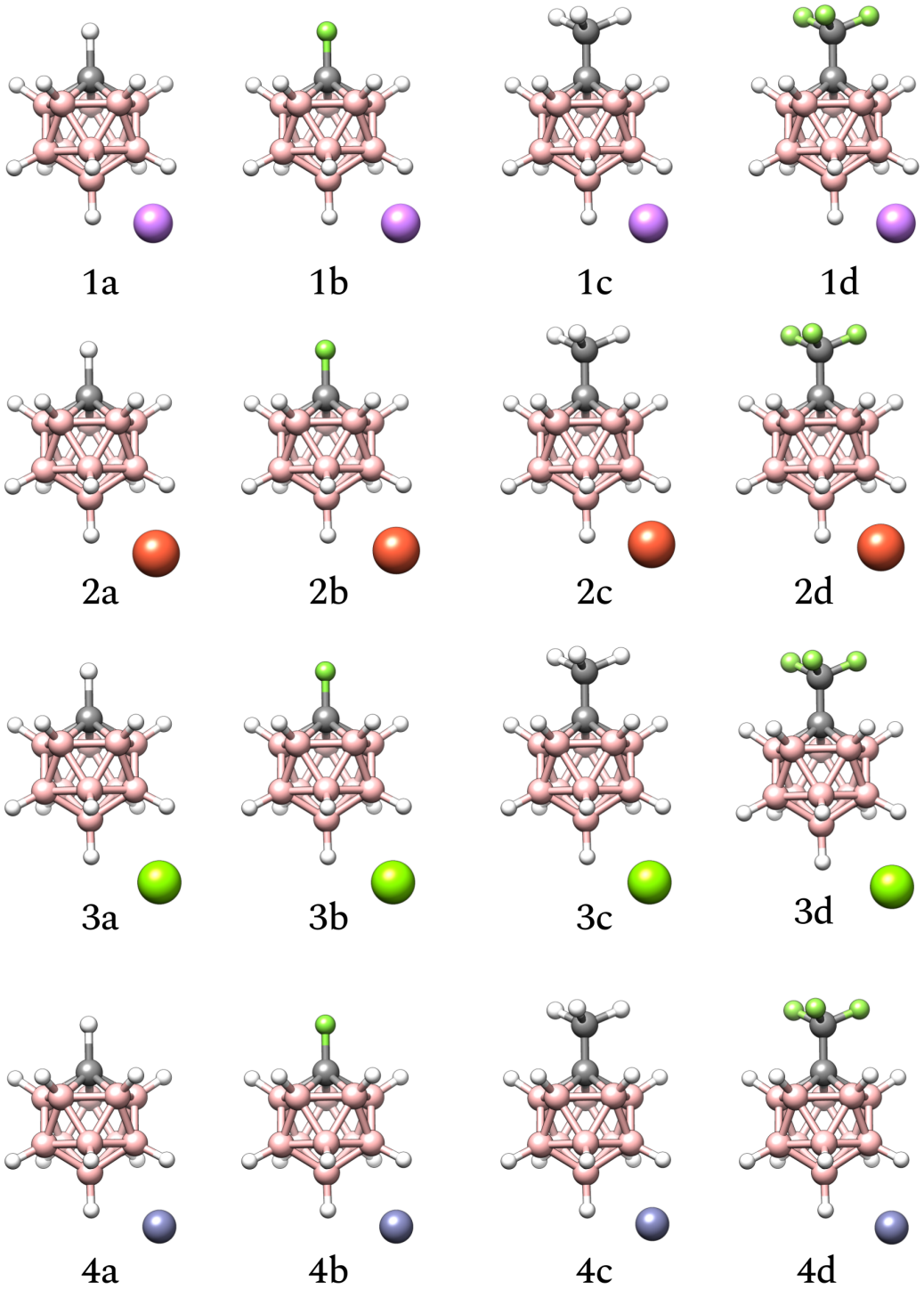


Figure S1: Structures of studied ion pair complexes **1a-4d**, $R{-}CB_{11}H_{11}^{-} \longleftrightarrow M^{q+}$ ($R = H, F, CH_3, CF_3$ and $M^{q+} = Li^+, Na^+, Mg^{2+}, Zn^{2+}$ in which the different R are represented by letters **a-d**, while the metallic cations $M^{q+}$ are denoted by the numbers **1-4**, respectively.

Table S1: Relative energies of the optimized structures ($\Delta E^{opt}$) reported in kcal $\cdot$ mol$^{-1}$ to evaluate the most stable coordination position (CP). As a reference, the coordinate structure at position 4, which has the lowest associated energies, is used.

| | | Relative energies ($\Delta E^{opt}$/ (kcal $\cdot$ mol$^{-1}$)) | | | |
|---|---|---|---|---|---|
| M | CP | (**1a**) | (**1b**) | (**1c**) | (**1d**) |
| $Li^{+}$ | 1 | 40.74 | 21.32 | 38.40 | 30.68 |
| | 2 | 20.09 | 10.43 | 23.84 | 8.76 |
| | 3 | 6.56 | 3.52 | 4.01 | 2.08 |
| | 4 | 0.00 | 0.00 | 0.00 | 0.00 |
| | 5 | 25.07 | 12.22 | 32.05 | 19.04 |
| $Na^{+}$ | 1 | 25.25 | 0.675 | 17.67 | 20.02 |
| | 2 | 1.02 | 0.900 | 0.982 | 1.01 |
| | 3 | 8.98 | 10.84 | 11.66 | 9.76 |
| | 4 | 0.00 | 0.00 | 0.00 | 0.00 |
| | 5 | 39.77 | 15.49 | 29.43 | 32.16 |
| $Mg^{+2}$ | 1 | 58.31 | 44.18 | 50.50 | 52.63 |
| | 2 | 28.15 | 29.99 | 27.68 | 25.51 |
| | 3 | 13.07 | 10.46 | 9.65 | 12.03 |
| | 4 | 0.00 | 0.00 | 0.00 | 0.00 |
| | 5 | 36.22 | 30.81 | 35.76 | 38.78 |
| $Zn^{+2}$ | 1 | 54.89 | 60.12 | 59.77 | 58.11 |
| | 2 | 35.02 | 30.75 | 26.10 | 28.45 |
| | 3 | 5.06 | 6.97 | 3.84 | 4.84 |
| | 4 | 0.00 | 0.00 | 0.00 | 0.00 |
| | 5 | 37.03 | 26.56 | 28.94 | 30.89 |

Table S2: Results of Energy Decomposition Analyses of closocarborane (**1a - 4a**), substituted with hydrogen at the apical position. The numbers in the C.P. column. (*cationic position*) indicate the position of the cations in the geometry of the complex.

| (**1a**) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C.P. | M | $\Delta E^{tot}$ | $\Delta E^{prep}$ | $\Delta E^{int}$ | $\Delta E^{elstat}$ | $\Delta E^{orb}$ | $\Delta E^{disp}$ | $\Delta E^{Pauli}$ |
| 1 | $Li^{+}$ | -60.40 | 8.91 | -69.31 | -53.47 | -20.26 | -0.64 | 5.06 |
| | $Na^{+}$ | -52.37 | 10.1 | -62.49 | -50.81 | -13.49 | -0.54 | 2.34 |
| | $Mg^{+2}$ | -179.19 | 6.78 | -185.97 | -100.77 | -85.85 | -1.61 | 2.26 |
| | $Zn^{+2}$ | -249.27 | 6.89 | -256.16 | -101.97 | -154.50 | -1.59 | 1.91 |
| 2 | $Li^{+}$ | -88.75 | 5.65 | -94.40 | -80.01 | -20.22 | -1.18 | 7.06 |
| | $Na^{+}$ | -76.03 | 6.81 | -82.84 | -84.43 | -15.70 | -0.84 | 18.14 |
| | $Mg^{+2}$ | -220.82 | 8.68 | -229.50 | -162.12 | -82.42 | -2.39 | 17.43 |
| | $Zn^{+2}$ | -275.99 | 8.31 | -284.30 | -171.04 | -131.27 | -2.27 | 20.25 |
| 3 | $Li^{+}$ | -106.98 | 6.13 | -113.11 | -95.29 | -42.50 | -1.56 | 25.02 |
| | $Na^{+}$ | -65.29 | 5.88 | -71.17 | -113.32 | -34.14 | -0.85 | 77.35 |
| | $Mg^{+2}$ | -275.39 | 8.13 | -283.52 | -198.83 | -152.23 | -2.26 | 71.50 |
| | $Zn^{+2}$ | -336.47 | 8.19 | -344.66 | -237.72 | -199.07 | -2.64 | 94.73 |
| 4 | $Li^{+}$ | -117.09 | 5.46 | -122.55 | -101.75 | -39.01 | -1.59 | 20.60 |
| | $Na^{+}$ | -79.87 | 7.65 | -87.52 | -115.77 | -31.85 | -0.75 | 61.22 |
| | $Mg^{+2}$ | -295.00 | 7.51 | -302.51 | -209.88 | -145.05 | -2.24 | 57.01 |
| | $Zn^{+2}$ | -351.92 | 8.43 | -360.35 | -240.87 | -191.92 | -2.58 | 72.09 |
| 5 | $Li^{+}$ | -77.45 | 6.71 | -84.16 | -85.21 | -37.79 | -1.47 | 40.31 |
| | $Na^{+}$ | -26.94 | 4.13 | -31.07 | -112.33 | -28.02 | -0.55 | 109.83 |
| | $Mg^{+2}$ | -203.76 | 6.77 | -210.53 | -183.69 | -126.18 | -2.41 | 101.75 |
| | $Zn^{+2}$ | -266.79 | 8.52 | -275.31 | -235.24 | -175.61 | -2.87 | 138.45 |

Table S3: Results of Energy Decomposition Analyses of closocarborane (**1b-4b**), substituted with hydrogen at the apical position. The numbers in the C.P. column. (*cationic position*) indicate the position of the cations in the geometry of the complex.

| (**1b**) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C.P. | M | $\Delta E^{tot}$ | $\Delta E^{prep}$ | $\Delta E^{int}$ | $\Delta E^{elstat}$ | $\Delta E^{orb}$ | $\Delta E^{disp}$ | $\Delta E^{Pauli}$ |
| 1 | $Li^{+}$ | -75.54 | 9.11 | -84.65 | -72.48 | -12.80 | -0.76 | 1.39 |
| | $Na^{+}$ | -73.11 | 8.23 | -81.34 | -73.48 | -11.70 | -0.84 | 4.77 |
| | $Mg^{+2}$ | -190.54 | 5.56 | -196.19 | -145.36 | -53.49 | -0.91 | 4.16 |
| | $Zn^{+2}$ | -236.98 | 7.19 | -244.17 | -148.31 | -100.40 | -1.47 | 6.05 |
| 2 | $Li^{+}$ | -84.93 | 5.48 | -90.41 | -76.08 | -20.03 | -1.16 | 6.88 |
| | $Na^{+}$ | -71.86 | 7.15 | -79.01 | -80.39 | -15.55 | -0.81 | 17.76 |
| | $Mg^{+2}$ | -211.23 | 9.12 | -220.35 | -154.20 | -80.80 | -2.39 | 17.03 |
| | $Zn^{+2}$ | -260.45 | 8.97 | -269.42 | -166.71 | -124.06 | -2.24 | 19.78 |
| 3 | $Li^{+}$ | -101.00 | 6.78 | -107.78 | -90.00 | -42.15 | -1.55 | 25.93 |
| | $Na^{+}$ | -61.91 | 4.21 | -66.12 | -107.83 | -33.91 | -0.85 | 76.42 |
| | $Mg^{+2}$ | -263.28 | 9.02 | -272.30 | -188.15 | -11.69 | -2.25 | 69.79 |
| | $Zn^{+2}$ | -321.86 | 10.87 | -332.73 | -226.63 | -197.92 | -2.64 | 93.85 |
| 4 | $Li^{+}$ | -110.45 | 6.79 | -117.24 | -96.67 | -39.44 | -1.59 | 20.46 |
| | $Na^{+}$ | -75.17 | 7.22 | -82.39 | -110.57 | -31.96 | -0.75 | 60.89 |
| | $Mg^{+2}$ | -283.21 | 8.12 | -291.33 | -199.61 | -159.61 | -2.10 | 55.72 |
| | $Zn^{+2}$ | -339.65 | 9.03 | -348.68 | -230.43 | -198.75 | -2.57 | 72.72 |
| 5 | $Li^{+}$ | -81.86 | 5.67 | -87.53 | -88.63 | -36.87 | -1.62 | 39.59 |
| | $Na^{+}$ | -30.25 | 5.55 | -35.80 | -115.20 | -27.96 | -0.95 | 108.31 |
| | $Mg^{+2}$ | -208.65 | 7.43 | -216.08 | -190.22 | -123.52 | -2.36 | 100.01 |
| | $Zn^{+2}$ | -268.26 | 8.01 | -276.2 | -241.18 | -169.69 | -2.65 | 137.25 |

Table S4: Results of Energy Decomposition Analyses of closocarborane (**1c-4c**), substituted with hydrogen at the apical position. The numbers in the column C.P. (cationic position) indicate the position of the cations in the geometry of the complex.

| (**1c**) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C.P. | M | $\Delta E^{tot}$ | $\Delta E^{prep}$ | $\Delta E^{int}$ | $\Delta E^{elstat}$ | $\Delta E^{orb}$ | $\Delta E^{disp}$ | $\Delta E^{Pauli}$ |
| 1 | $Li^{+}$ | -61.43 | 7.88 | -69.31 | -53.47 | -20.03 | -1.16 | 6.88 |
| | $Na^{+}$ | -48.59 | 9.11 | -57.70 | -56.97 | -16.76 | -0.74 | 16.78 |
| | $Mg^{+2}$ | -167.81 | 9.23 | -177.04 | -108.40 | -82.37 | -1.12 | 14.85 |
| | $Zn^{+2}$ | -226.98 | 8.25 | -235.23 | -117.02 | -136.87 | -1.21 | 19.87 |
| 2 | $Li^{+}$ | -89.51 | 6.12 | -95.63 | -81.19 | -20.36 | -1.19 | 7.12 |
| | $Na^{+}$ | -78.04 | 5.99 | -84.03 | -85.65 | -15.78 | -0.85 | 18.25 |
| | $Mg^{+2}$ | -223.85 | 8.22 | -232.07 | -164.50 | -82.72 | -2.40 | 17.54 |
| | $Zn^{+2}$ | -277.94 | 7.83 | -285.77 | -173.49 | -130.42 | -2.25 | 20.39 |
| 3 | $Li^{+}$ | -106.93 | 7.16 | -114.09 | -95.95 | -42.74 | -1.62 | 26.22 |
| | $Na^{+}$ | -64.67 | 7.48 | -72.15 | -113.95 | -34.34 | -0.96 | 77.10 |
| | $Mg^{+2}$ | -276.06 | 9.80 | -285.87 | -200.13 | -153.82 | -2.37 | 70.45 |
| | $Zn^{+2}$ | -338.30 | 8.97 | -347.27 | -238.97 | -200.18 | -2.75 | 94.62 |
| 4 | $Li^{+}$ | -116.50 | 7.40 | -124.13 | -103.31 | -39.92 | -1.61 | 20.72 |
| | $Na^{+}$ | -82.33 | 6.68 | -89.01 | -117.39 | -32.33 | -0.77 | 61.48 |
| | $Mg^{+2}$ | -299.22 | 6.71 | -305.93 | -213.00 | -147.00 | -2.26 | 56.33 |
| | $Zn^{+2}$ | -355.04 | 7.13 | -362.17 | -244.14 | -190.84 | -2.59 | 73.41 |
| 5 | $Li^{+}$ | -77.38 | 5.09 | -82.47 | -83.30 | -41.00 | -1.57 | 43.40 |
| | $Na^{+}$ | -22.58 | 4.15 | -26.73 | -112.43 | -31.28 | -0.91 | 117.88 |
| | $Mg^{+2}$ | -204.96 | 6.78 | -211.74 | -180.78 | -137.54 | -2.65 | 109.24 |
| | $Zn^{+2}$ | -269.20 | 7.81 | -277.01 | -237.05 | -186.84 | -3.02 | 149.90 |

Table S5: Results of Energy Decomposition Analyses of closocarborane (**1d-4d**), substituted with hydrogen at the apical position. The numbers in the column C.P. (cationic position) indicate the position of the cations in the geometry of the complex.

| (**1d**) | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| C.P. | M | $\Delta E^{tot}$ | $\Delta E^{prep}$ | $\Delta E^{int}$ | $\Delta E^{elstat}$ | $\Delta E^{orb}$ | $\Delta E^{disp}$ | $\Delta E^{Pauli}$ |
| 1 | $Li^{+}$ | -56.83 | 7.99 | -64.82 | -51.04 | -21.36 | -0.77 | 8.40 |
| | $Na^{+}$ | -38.34 | 9.18 | -47.52 | -57.41 | -18.28 | -0.90 | 29.06 |
| | $Mg^{+2}$ | -156.22 | 8.54 | -164.76 | -104.68 | -83.60 | -1.03 | 24.55 |
| | $Zn^{+2}$ | -202.69 | 7.98 | -210.67 | -122.18 | -131.21 | -1.06 | 43.78 |
| 2 | $Li^{+}$ | -88.64 | 5.42 | -94.06 | -79.58 | -20.33 | -1.19 | 7.04 |
| | $Na^{+}$ | -76.23 | 6.23 | -82.52 | -83.99 | -15.78 | -0.85 | 18.10 |
| | $Mg^{+2}$ | -221.86 | 6.79 | -228.65 | -161.25 | -82.39 | -2.40 | 17.39 |
| | $Zn^{+2}$ | -273.77 | 8.91 | -282.68 | -170.16 | -130.48 | -2.25 | 20.21 |
| 3 | $Li^{+}$ | -105.23 | 6.71 | -111.94 | -93.69 | -42.66 | -1.64 | 26.05 |
| | $Na^{+}$ | -64.93 | 5.23 | -70.16 | -111.58 | -34.31 | -0.99 | 76.72 |
| | $Mg^{+2}$ | -272.33 | 8.99 | -281.32 | -195.56 | -153.42 | -2.39 | 70.05 |
| | $Zn^{+2}$ | -333.36 | 9.01 | -342.37 | -234.18 | -199.54 | -2.78 | 94.13 |
| 4 | $Li^{+}$ | -114.43 | 7.48 | -121.91 | -101.08 | -39.83 | -1.61 | 20.61 |
| | $Na^{+}$ | -79.66 | 7.23 | -86.89 | -115.08 | -32.27 | -0.77 | 61.24 |
| | $Mg^{+2}$ | -293.02 | 8.14 | -301.16 | -208.49 | -146.48 | -2.27 | 56.08 |
| | $Zn^{+2}$ | -350.52 | 8.45 | -358.97 | -239.49 | -189.99 | -2.60 | 73.12 |
| 5 | $Li^{+}$ | -73.78 | 4.07 | -77.85 | -78.68 | -41.69 | -1.79 | 44.31 |
| | $Na^{+}$ | -14.41 | 4.98 | -19.40 | -108.68 | -31.98 | -1.22 | 122.47 |
| | $Mg^{+2}$ | -194.67 | 5.67 | -200.34 | -171.83 | -138.57 | -2.52 | 112.58 |
| | $Zn^{+2}$ | -255.97 | 8.19 | -264.16 | -231.38 | -186.47 | -2.85 | 158.54 |

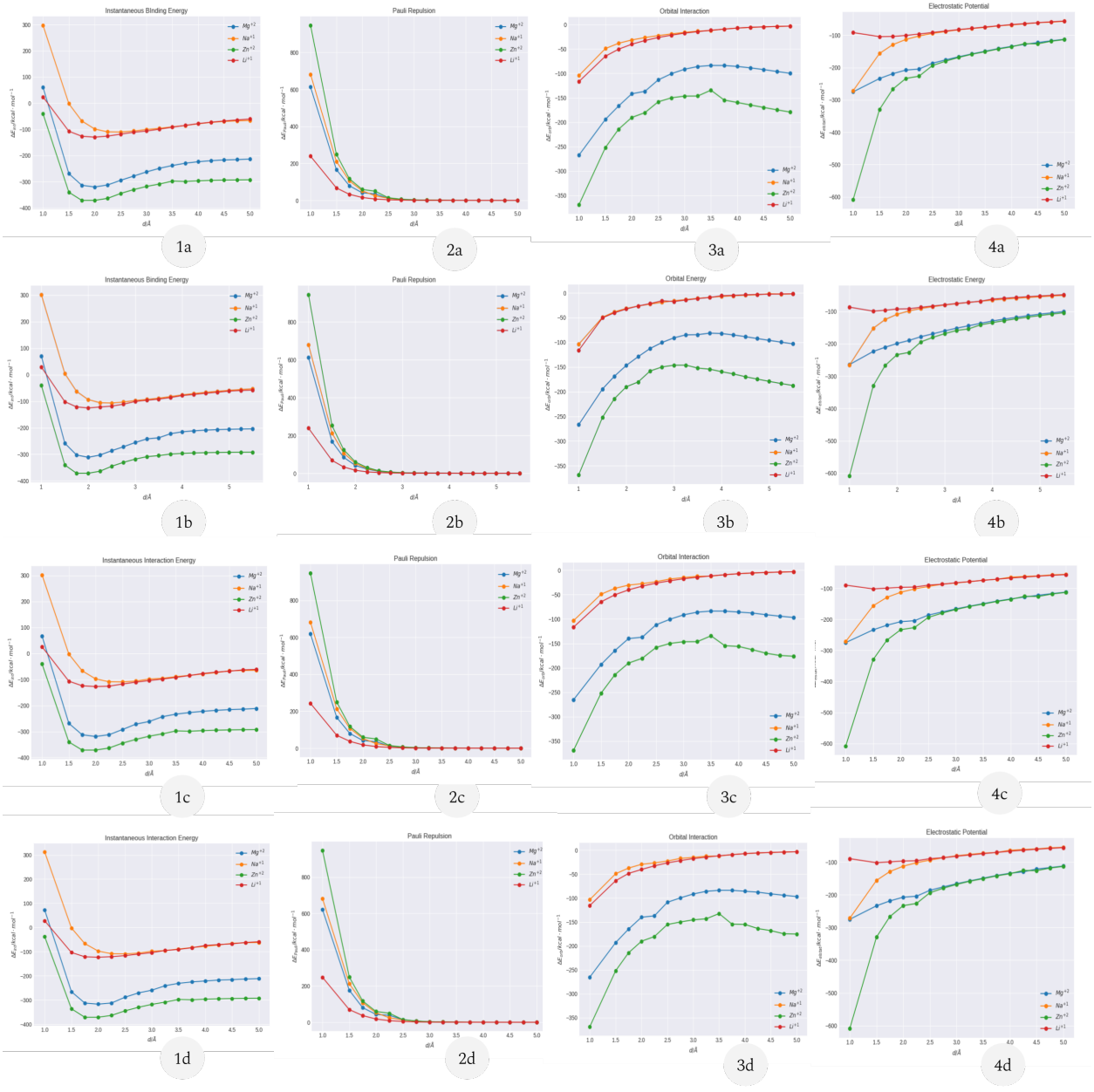


Figure S2: Graphs of the rigid molecular scans. The labels on the graphs correspond to the plotted EDA terms. The **1a-1d** plots refer to the $\Delta E^{int}$ values for the anions substituted, respectively, by: $H, F, CH_3, CF_3$. The **2a-2d** plots follow the same order of anionic substitution, representing Pauli repulsion ($\Delta E^{Pauli}$). The **3a-3d** plots follow the same order of anionic substitution, representing the orbital interaction ($\Delta E^{orb}$). The **4a-4d** graphs follow the same order of anionic substitution, representing the electrostatic interaction ($\Delta E^{elstat}$).

Table S6: Charge Transfer Integrals calculations results, following the numbering scheme of figure 2.

| | | HOMO(Fragment 1)⟶LUMO(Fragment 2) | | | | | LUMO(Fragment 1)⟶HOMO(Fragment 2) | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| M | | e1/(eV) | e2/(eV) | S | J/(eV) | V/(eV) | e1/(eV) | e2/(eV) | S | J/(eV) | V/(eV) |
| $Li^+$ | 1a | -54.62 | -1.170 | -0.008 | 0.451 | 0.216 | -4.100 | -8.020 | -0.040 | -0.4179 | 0.1770 |
| | 1b | -52.11 | -1.138 | -0.006 | 0.412 | 0.201 | -4.001 | -8.008 | -0.030 | -0.4007 | 0.1601 |
| | 1c | -47.07 | -0.917 | -0.007 | 0.438 | 0.188 | -4.077 | -7.815 | -0.022 | -0.360 | -0.1489 |
| | 1d | -48.99 | -0.877 | -0.011 | 0.455 | 0.193 | -4.153 | -7.926 | -0.027 | -0.343 | -0.142 |
| $Na^+$ | 1a | -31.80 | -1.152 | -0.001 | 0.009 | 0.005 | -3.977 | -7.992 | -0.426 | -0.042 | -0.179 |
| | 1b | -29.86 | -1.148 | 0 | 0.007 | 0.003 | -3.702 | -7.788 | -0.395 | -0.033 | -0.1602 |
| | 1c | -36.06 | -1.216 | -0.0047 | 0.012 | 0.0064 | -4.167 | -8.204 | -0.552 | -0.061 | -0.222 |
| | 1d | -32.04 | -1.199 | -0.003 | 0.008 | 0.008 | -4.014 | -8.001 | -0.473 | -0.056 | -0.194 |
| $Mg^{+2}$ | 1a | -7.671 | -1.494 | -0.054 | 0.421 | 0.173 | -4.145 | -8.424 | 0.040 | -0.466 | -0.215 |
| | 1b | -7.589 | -1.432 | -0.045 | 0.388 | 0.162 | -4.076 | -8.403 | 0.039 | -0.459 | -0.201 |
| | 1c | -7.412 | -1.377 | -0.038 | 0.400 | 0.177 | -4.113 | -8.255 | 0.032 | -0.440 | -0.171 |
| | 1d | -7.625 | -1.521 | -0.053 | 0.350 | 0.129 | -4.094 | -8.547 | 0.0297 | -0.418 | -0.188 |
| $Zn^{+2}$ | 1a | -8.678 | -1.836 | -0.046 | 0.423 | 0.178 | -2.894 | -8.741 | -0.034 | 0.411 | 0.211 |
| | 1b | -8.501 | -1.789 | -0.045 | 0.599 | 0.181 | -2.520 | -8.312 | -0.020 | 0.509 | 0.379 |
| | 1c | -8.101 | -1.068 | -0.024 | 0.822 | 0.235 | -2.929 | -8.784 | -0.079 | 0.896 | 0.555 |
| | 1d | -8.998 | -1.820 | -0.017 | 0.733 | 0.302 | -3.001 | -9.007 | -0.101 | 0.708 | 0.312 |

Table S7: Cartesian coordinates of complex (**1a**)

C 2.352162390 8.107331315 13.247610618 B 4.789502499 7.205244081 14.151662747 H 5.448506089 6.398

Table S8: Cartesian coordinates of complex (**2a**)

| | | | |
|---|---|---|---|
| C | 2.343567982 | 8.098992583 | 13.252900281 |
| B | 4.782596273 | 7.199442840 | 14.154925671 |
| H | 5.441774967 | 6.391175467 | 14.714170127 |
| B | 3.237525215 | 7.928674780 | 11.815090051 |
| H | 2.695956168 | 7.619546569 | 10.811529574 |
| B | 2.866419215 | 9.346587302 | 14.289703623 |
| H | 2.073730831 | 9.969652921 | 14.906137353 |
| B | 3.378986117 | 6.747981785 | 13.157674928 |
| H | 2.923885532 | 5.667252676 | 13.019317731 |
| B | 2.923219064 | 9.527832147 | 12.524752710 |
| H | 2.169656282 | 10.266678641 | 11.990480154 |
| B | 4.554929289 | 9.119440984 | 11.964688222 |
| H | 5.047842976 | 9.643075979 | 11.002805736 |
| B | 4.456430732 | 8.820243961 | 14.854846465 |
| H | 4.876577978 | 9.144715701 | 15.914188799 |
| B | 4.319355192 | 9.998496863 | 13.511838119 |
| H | 4.632582615 | 11.151310381 | 13.638943996 |
| B | 3.149604079 | 7.628600475 | 14.678279435 |
| H | 2.532882275 | 7.135896984 | 15.557420095 |
| B | 4.823853464 | 7.395540262 | 12.372907746 |
| B | 5.488638671 | 8.663552715 | 13.418448776 |
| H | 6.676843093 | 8.862172140 | 13.477691720 |
| H | 5.517461783 | 6.718243114 | 11.689855773 |
| H | 1.280875622 | 7.924437243 | 13.199023291 |
| Na | 6.497321863 | 10.766226001 | 12.367179324 |

Table S9: Cartesian coordinates of complex (**3a**)

| | | | |
|---|---|---|---|
| C | 2.343129560 | 8.099687677 | 13.250643508 |
| B | 4.780282873 | 7.197303342 | 14.154902672 |
| H | 5.456710119 | 6.406130355 | 14.706602302 |
| B | 3.238904486 | 7.930408486 | 11.813842235 |
| H | 2.721063093 | 7.639542990 | 10.798717730 |
| B | 2.865485778 | 9.345682429 | 14.289618156 |
| H | 2.093685547 | 9.988404170 | 14.902140243 |
| B | 3.377693697 | 6.748036241 | 13.155227604 |
| H | 2.939102132 | 5.667761776 | 13.007049107 |
| B | 2.924801631 | 9.528959421 | 12.524959880 |
| H | 2.199469922 | 10.284336599 | 11.986083483 |
| B | 4.556969829 | 9.120038776 | 11.966619105 |
| H | 5.105425229 | 9.688357021 | 11.020267104 |
| B | 4.454349573 | 8.817518029 | 14.856287884 |
| H | 4.886521254 | 9.154596756 | 15.901182984 |
| B | 4.319944499 | 9.997447536 | 13.514482128 |
| H | 4.697179019 | 11.167611646 | 13.610146594 |
| B | 3.146897336 | 7.627034527 | 14.676555500 |
| H | 2.543565203 | 7.143068884 | 15.562264445 |
| B | 4.824089909 | 7.395464248 | 12.373173906 |
| B | 5.488382985 | 8.661763088 | 13.421101844 |
| H | 6.705176994 | 8.921098755 | 13.450645073 |
| H | 5.529004630 | 6.739873629 | 11.688807498 |
| H | 1.278557263 | 7.936370577 | 13.188158901 |
| Mg | 6.216124717 | 10.529273554 | 12.465319815 |

Table S10: Cartesian coordinates of complex (**4a**)

| | | | |
|---|---|---|---|
| C | 2.345223726 | 8.102753909 | 13.248903143 |
| B | 4.782596818 | 7.200769408 | 14.152968885 |
| H | 5.456863085 | 6.408756671 | 14.704684829 |
| B | 3.240997133 | 7.933873978 | 11.812053964 |
| H | 2.723817875 | 7.639998242 | 10.798207337 |
| B | 2.867337240 | 9.348713772 | 14.288041585 |
| H | 2.095835198 | 9.988197775 | 14.903135543 |
| B | 3.380078547 | 6.751340582 | 13.153267010 |
| H | 2.947616486 | 5.669727551 | 13.000119021 |
| B | 2.926566409 | 9.532255246 | 12.523407895 |
| H | 2.201797814 | 10.287245969 | 11.984865336 |
| B | 4.558808494 | 9.123768325 | 11.964965445 |
| H | 5.101197264 | 9.672797186 | 10.993626573 |
| B | 4.456330652 | 8.820813306 | 14.854593793 |
| H | 4.884237376 | 9.156118420 | 15.901061174 |
| B | 4.321633910 | 10.000904936 | 13.512959877 |
| H | 4.685673734 | 11.181350438 | 13.635978525 |
| B | 3.149131946 | 7.630071816 | 14.674726367 |
| H | 2.550565294 | 7.150375971 | 15.565418074 |
| B | 4.826313511 | 7.399193883 | 12.371267224 |
| B | 5.490359690 | 8.665487377 | 13.419358100 |
| H | 6.728608517 | 8.921692669 | 13.456296047 |
| H | 5.527146793 | 6.740734223 | 11.686584767 |
| H | 1.280212301 | 7.940070548 | 13.185862171 |
| Zn | 6.163567466 | 10.468758313 | 12.492447014 |

Table S11: Cartesian coordinates of complex (**1b**)

| | | | |
|---|---|---|---|
| C | 2.368694432 | 8.109789559 | 13.249119943 |
| B | 4.806582035 | 7.208597142 | 14.152588087 |
| H | 5.459775027 | 6.398290986 | 14.711944811 |
| B | 3.263933194 | 7.940494043 | 11.811986462 |
| H | 2.708080429 | 7.633800102 | 10.818753186 |
| B | 2.890995663 | 9.356256689 | 14.287555484 |
| H | 2.085685484 | 9.968260174 | 14.893583495 |
| B | 3.403750698 | 6.758521098 | 13.153616929 |
| H | 2.931959679 | 5.687823292 | 13.014311869 |
| B | 2.949499121 | 9.539103771 | 12.522825493 |
| H | 2.184811991 | 0.265537547 | 11.993790127 |
| B | 4.581593899 | 9.130682385 | 11.963904954 |
| H | 5.100015540 | 9.681141529 | 11.028796888 |
| B | 4.480304900 | 8.828863467 | 14.853694087 |
| H | 4.894334366 | 9.153423414 | 15.913032653 |
| B | 4.344872320 | 0.008395289 | 13.511642022 |
| H | 4.694649776 | 1.155467190 | 13.612663250 |
| B | 3.173246337 | 7.637819160 | 14.674815852 |
| H | 2.540779679 | 7.147327016 | 15.540483742 |
| B | 4.849563658 | 7.406317648 | 12.370790294 |
| B | 5.513797482 | 8.673147049 | 13.418114361 |
| H | 6.696205714 | 8.916847876 | 13.449968181 |
| H | 5.538718310 | 6.729487149 | 11.685980655 |
| F | 1.008964872 | 7.886362048 | 13.174182218 |
| Li | 6.221702675 | 0.514014890 | 12.476654658 |

Table S12: Cartesian coordinates of complex (**2b**)

| | | | |
|---|---|---|---|
| C | 2.360102543 | 8.100951638 | 13.254925533 |
| B | 4.800125206 | 7.203137513 | 14.155990293 |
| H | 5.454188938 | 6.392395023 | 14.715822126 |
| B | 3.253308659 | 7.930356286 | 11.816681456 |
| H | 2.692322321 | 7.619002585 | 10.826692623 |
| B | 2.882909334 | 9.349353793 | 14.290778953 |
| H | 2.074411873 | 9.958011183 | 14.897655081 |
| B | 3.396168283 | 6.750430867 | 13.159792913 |
| H | 2.922222776 | 5.679679948 | 13.021344245 |
| B | 2.938584222 | 9.529716322 | 12.525701810 |
| H | 2.168449673 | 10.252753805 | 11.997717585 |
| B | 4.570179564 | 9.121885115 | 11.964895166 |
| H | 5.058938124 | 9.645325064 | 11.001933363 |
| B | 4.473524439 | 8.824130056 | 14.855264540 |
| H | 4.888153802 | 9.148248221 | 15.915863469 |
| B | 4.335051191 | 10.001617467 | 13.511728316 |
| H | 4.642108926 | 11.155106772 | 13.638995890 |
| B | 3.167215625 | 7.631715553 | 14.680076262 |
| H | 2.533701899 | 7.142077997 | 15.546593233 |
| B | 4.840239744 | 7.398335691 | 12.373847559 |
| B | 5.504974930 | 8.667233948 | 13.418345205 |
| H | 6.691555656 | 8.863416795 | 13.478485478 |
| H | 5.528101698 | 6.718112396 | 11.689347395 |
| F | 1.000452652 | 7.876256898 | 13.182369060 |
| Na | 6.515525200 | 10.776519578 | 12.363952148 |

Table S13: Cartesian coordinates of complex (**3b**)

| | | | |
|---|---|---|---|
| C | 2.359727436 | 8.102904152 | 13.251702234 |
| B | 4.797333089 | 7.201265393 | 14.155485728 |
| H | 5.467945621 | 6.406578870 | 14.708288077 |
| B | 3.255169761 | 7.933589563 | 11.814697818 |
| H | 2.717851635 | 7.640437341 | 10.811456745 |
| B | 2.882053243 | 9.349206461 | 14.290323234 |
| H | 2.093650594 | 9.978235569 | 14.894250325 |
| B | 3.394592538 | 6.751485429 | 13.156253777 |
| H | 2.937708699 | 5.679759354 | 13.007150103 |
| B | 2.940866365 | 9.532189110 | 12.525617583 |
| H | 2.199353226 | 10.273749046 | 11.991948899 |
| B | 4.572987937 | 9.123564204 | 11.966924148 |
| H | 5.115059048 | 9.692059575 | 11.018805074 |
| B | 4.471191504 | 8.821524125 | 14.856672344 |
| H | 4.897278973 | 9.157513514 | 15.903835417 |
| B | 4.336153342 | 10.001186512 | 13.514695292 |
| H | 4.706514078 | 11.171901267 | 13.609764021 |
| B | 3.163979619 | 7.630694130 | 14.677487902 |
| H | 2.543817505 | 7.149699664 | 15.552089635 |
| B | 4.840629366 | 7.399125228 | 12.373711021 |
| B | 5.504889458 | 8.665767391 | 13.421244866 |
| H | 6.718811813 | 8.917516787 | 13.454599174 |
| H | 5.539616427 | 6.739806962 | 11.687741967 |
| F | 0.999975748 | 7.879690472 | 13.176529147 |
| Mg | 6.235360254 | 10.536320395 | 12.463525169 |

Table S14: Cartesian coordinates of complex (**4b**)

| | | | |
|---|---|---|---|
| C | 2.362315975 | 8.106409439 | 13.249781598 |
| B | 4.800338419 | 7.205524681 | 14.153192717 |
| H | 5.467911053 | 6.409397648 | 14.706160188 |
| B | 3.257680155 | 7.937637133 | 11.812664713 |
| H | 2.720645201 | 7.641704802 | 10.810757325 |
| B | 2.884288074 | 9.352746470 | 14.288538732 |
| H | 2.095811564 | 9.978551789 | 14.894654801 |
| B | 3.397664828 | 6.755382759 | 13.154029754 |
| H | 2.948504469 | 5.681480891 | 12.999450516 |
| B | 2.942862676 | 9.536015220 | 12.523854841 |
| H | 2.201631547 | 10.277008508 | 11.990572439 |
| B | 4.575078883 | 9.128069687 | 11.964941354 |
| H | 5.103691515 | 9.678255838 | 10.990472097 |
| B | 4.473673886 | 8.825559115 | 14.854654101 |
| H | 4.895400739 | 9.159224334 | 15.903565553 |
| B | 4.338074683 | 10.005373389 | 13.512867165 |
| H | 4.688644773 | 11.187148003 | 13.633003750 |
| B | 3.166879171 | 7.634279088 | 14.675418175 |
| H | 2.552739689 | 7.157664357 | 15.556252355 |
| B | 4.843389099 | 7.403667521 | 12.371443504 |
| B | 5.507288909 | 8.670394872 | 13.419102737 |
| H | 6.741007758 | 8.906063445 | 13.466859380 |
| H | 5.538085230 | 6.741062698 | 11.685453276 |
| F | 1.002638515 | 7.882710880 | 13.174707290 |
| Zn | 6.186270467 | 10.474437946 | 12.492401338 |

Table S15: Cartesian coordinates of complex (**1c**)

| | | | |
|---|---|---|---|
| C | 2.352311568 | 8.132107917 | 13.210259833 |
| B | 4.792512079 | 7.252098274 | 14.128248365 |
| H | 5.483283997 | 6.468839496 | 14.728574772 |
| B | 3.256524679 | 7.967557669 | 11.778202613 |
| H | 2.711058183 | 7.636750849 | 10.785082505 |
| B | 2.859043773 | 9.384510870 | 14.249267280 |
| H | 2.054765039 | 9.978634675 | 14.877452104 |
| B | 3.398683104 | 6.789045699 | 13.122628806 |
| H | 2.951869170 | 5.702920706 | 13.005509354 |
| B | 2.925476940 | 9.564801424 | 12.484554956 |
| H | 2.151837081 | 10.283539903 | 11.955074994 |
| B | 4.563754261 | 9.168562565 | 11.935031647 |
| H | 5.067750558 | 9.680316373 | 10.995985880 |
| B | 4.449499723 | 8.870886075 | 14.824766914 |
| H | 4.902003657 | 9.162470620 | 15.903550334 |
| B | 4.311747876 | 10.046991498 | 13.479946715 |
| H | 4.627509637 | 11.178653125 | 13.625705806 |
| B | 3.153022304 | 7.669064281 | 14.641036373 |
| H | 2.540679205 | 7.165985225 | 15.517793597 |
| B | 4.843395580 | 7.447107677 | 12.346359940 |
| B | 5.491842858 | 8.721028898 | 13.394974193 |
| H | 6.680836319 | 8.916044547 | 13.502526218 |
| H | 5.552738479 | 6.761523005 | 11.689777148 |
| C | 0.839121772 | 7.853035150 | 13.147211919 |
| H | 0.481169377 | 7.966121720 | 12.125320774 |
| H | 0.627880417 | 6.838108322 | 13.479212082 |
| H | 0.298637555 | 8.549490488 | 13.785000769 |
| Li | 6.479691247 | 8.117534824 | 15.234153930 |

Table S16: Cartesian coordinates of complex (**2c**)

| | | | |
|---|---|---|---|
| C | 2.357539980 | 8.133122275 | 13.227743523 |
| B | 4.783579833 | 7.273004963 | 14.102553561 |
| H | 5.459252978 | 6.476954483 | 14.713229760 |
| B | 3.283327926 | 7.965344267 | 11.792622563 |
| H | 2.737373343 | 7.643298589 | 10.795062537 |
| B | 2.875948002 | 9.398137095 | 14.262500129 |
| H | 2.087966643 | 10.008440729 | 14.897211160 |
| B | 3.418598921 | 6.796294856 | 13.117753188 |
| H | 2.978124745 | 5.705444655 | 13.003757002 |
| B | 2.939104551 | 9.563725054 | 12.496734578 |
| H | 2.163541101 | 10.276767471 | 11.956220523 |
| B | 4.575014967 | 9.161127557 | 11.949845976 |
| H | 5.057209864 | 9.680794599 | 10.997783929 |
| B | 4.450482129 | 8.869181203 | 14.801614346 |
| H | 4.894504020 | 9.160991813 | 15.888074216 |
| B | 4.324547460 | 10.046620407 | 13.480346707 |
| H | 4.635435321 | 11.183726758 | 13.624927425 |
| B | 3.156662842 | 7.678996875 | 14.650426324 |
| H | 2.558383468 | 7.166175936 | 15.534374680 |
| B | 4.873882334 | 7.441847189 | 12.339245904 |
| B | 5.500197184 | 8.727920545 | 13.380143185 |
| H | 6.690283515 | 8.929689484 | 13.489832459 |
| H | 5.570561667 | 6.742561263 | 11.677803251 |
| C | 0.856905601 | 7.853929425 | 13.143976355 |
| H | 0.395242815 | 7.987494088 | 11.896876139 |
| H | 0.562019852 | 6.610505424 | 13.543692415 |
| H | 0.151372164 | 8.689009152 | 13.915122468 |
| Na | 6.511583210 | 8.102625724 | 15.273735516 |

Table S17: Cartesian coordinates of complex (**3c**)

| | | | |
|---|---|---|---|
| C | 2.342943335 | 8.131893504 | 13.205858232 |
| B | 4.784587960 | 7.252391800 | 14.120487456 |
| H | 5.500992308 | 6.461217879 | 14.738307093 |
| B | 3.245203127 | 7.967482714 | 11.772553526 |
| H | 2.716893944 | 7.629897068 | 10.777778533 |
| B | 2.850867453 | 9.384425242 | 14.244128188 |
| H | 2.068629949 | 9.981259404 | 14.889433291 |
| B | 3.389458076 | 6.789035867 | 13.116813475 |
| H | 2.965815625 | 5.696829421 | 13.012529753 |
| B | 2.914818808 | 9.564680384 | 12.479320564 |
| H | 2.154270299 | 10.295479720 | 11.957561713 |
| B | 4.552411213 | 9.168750464 | 11.927537729 |
| H | 5.074570417 | 9.677960545 | 11.002373734 |
| B | 4.442221154 | 8.871130854 | 14.817436697 |
| H | 4.918011805 | 9.164635110 | 15.917966179 |
| B | 4.302372713 | 10.047172024 | 13.472776695 |
| H | 4.633295766 | 11.169289043 | 13.629880162 |
| B | 3.145728092 | 7.669047609 | 14.635536133 |
| H | 2.561825307 | 7.166030937 | 15.526382081 |
| B | 4.832962959 | 7.447362245 | 12.338524893 |
| B | 5.482611097 | 8.721440544 | 13.386204625 |
| H | 6.705063019 | 8.920846306 | 13.499116590 |
| H | 5.553061995 | 6.764632210 | 11.697423453 |
| C | 0.829722841 | 7.852519710 | 13.144915428 |
| H | 0.477258515 | 7.968491556 | 12.122015145 |
| H | 0.617763381 | 6.837379804 | 13.473225475 |
| H | 0.289816517 | 8.549457695 | 13.781422675 |
| Mg | 6.495468763 | 8.122992220 | 15.265700307 |

Table S18: Cartesian coordinates of complex (**4c**)

| | | | |
|---|---|---|---|
| C | 2.301347420 | 8.122508112 | 13.226865474 |
| B | 4.762784898 | 7.244436483 | 14.100845062 |
| H | 5.398494998 | 6.409033966 | 14.673718746 |
| B | 3.265718800 | 7.959760245 | 11.799737907 |
| H | 2.737982225 | 7.619279515 | 10.803354528 |
| B | 2.830774120 | 9.375291211 | 14.247261949 |
| H | 2.029722968 | 9.979206418 | 14.863793581 |
| B | 3.367854886 | 6.805108640 | 13.119551758 |
| H | 2.921286174 | 5.722373453 | 12.999474755 |
| B | 2.924333493 | 9.559282209 | 12.500842280 |
| H | 2.169095943 | 10.295000176 | 11.976420897 |
| B | 4.527794675 | 9.161613740 | 11.924864306 |
| H | 5.030898966 | 9.676497146 | 10.993132903 |
| B | 4.420620615 | 8.882130173 | 14.818012025 |
| H | 4.813607400 | 9.207551262 | 15.899525222 |
| B | 4.315152221 | 10.040952750 | 13.499995591 |
| H | 4.623914842 | 11.172127893 | 13.624990998 |
| B | 3.144606784 | 7.678050003 | 14.648278010 |
| H | 2.546707573 | 7.166982012 | 15.525318489 |
| B | 4.866012719 | 7.427537582 | 12.355882589 |
| B | 5.488201490 | 8.733486937 | 13.359460805 |
| H | 6.660920762 | 8.984917622 | 13.348358332 |
| H | 5.555601918 | 6.744075305 | 11.686664707 |
| C | 0.813033319 | 7.855256752 | 13.121472229 |
| H | 0.465537801 | 7.980843558 | 12.095874488 |
| H | 0.572520915 | 6.838104681 | 13.430262458 |
| H | 0.242164671 | 8.538372081 | 13.750141809 |
| Zn | 7.051953823 | 8.093951940 | 15.559107908 |

Table S19: Cartesian coordinates of complex (**1d**)

| | | | |
|---|---|---|---|
| C | 2.353335725 | 8.132352675 | 13.230757300 |
| B | 4.779529994 | 7.262150601 | 14.111006892 |
| H | 5.462079999 | 6.453949389 | 14.715649193 |
| B | 3.292659723 | 7.964217403 | 11.800244745 |
| H | 2.742580934 | 7.647529735 | 10.810886930 |
| B | 2.883987716 | 9.398523162 | 14.269453134 |
| H | 2.084393624 | 10.001693623 | 14.884237015 |
| B | 3.423968056 | 6.796013078 | 13.124090273 |
| H | 2.970590742 | 5.718195166 | 13.000407854 |
| B | 2.945523248 | 9.561943107 | 12.504971396 |
| H | 2.171886074 | 10.266317314 | 11.967029350 |
| B | 4.582169327 | 9.162888702 | 11.950383951 |
| H | 5.063029465 | 9.678619194 | 11.006635864 |
| B | 4.446343416 | 8.868707681 | 14.814726360 |
| H | 4.895819914 | 9.170490444 | 15.906112673 |
| B | 4.333241487 | 10.045887432 | 13.490555387 |
| H | 4.653903927 | 11.173692527 | 13.627849146 |
| B | 3.163331832 | 7.680576040 | 14.654305255 |
| H | 2.552620260 | 7.171013279 | 15.523360050 |
| B | 4.883409308 | 7.437407149 | 12.349874998 |
| B | 5.497632415 | 8.727627053 | 13.378337592 |
| H | 6.707538394 | 8.930832515 | 13.493281310 |
| H | 5.585045188 | 6.751266643 | 11.693584406 |
| C | 0.887764489 | 7.859430739 | 13.144099578 |
| F | 0.374967833 | 7.981641904 | 11.900420338 |
| F | 0.540727573 | 6.610821581 | 13.539673120 |
| F | 0.127439350 | 8.677389617 | 13.908918543 |
| Li | 6.443126414 | 8.142554114 | 15.152357152 |

Table S20: Cartesian coordinates of complex (**2d**)

| | | | |
|---|---|---|---|
| C | 2.344082370 | 8.133773564 | 13.222975680 |
| B | 4.776240370 | 7.265608540 | 14.108234180 |
| H | 5.462119387 | 6.458242405 | 14.713942551 |
| B | 3.282529901 | 7.965665008 | 11.793175409 |
| H | 2.733399429 | 7.646842096 | 10.803588541 |
| B | 2.877544737 | 9.397935680 | 14.262266257 |
| H | 2.079691151 | 10.002187015 | 14.879594075 |
| B | 3.416773396 | 6.799339179 | 13.118625054 |
| H | 2.966114985 | 5.719451906 | 12.996191877 |
| B | 2.935455081 | 9.562599201 | 12.497589621 |
| H | 2.162057856 | 10.268889085 | 11.961146003 |
| B | 4.571998864 | 9.162658432 | 11.946264826 |
| H | 5.057040770 | 9.678799819 | 11.003605860 |
| B | 4.444030805 | 8.867617638 | 14.809971337 |
| H | 4.896915756 | 9.169312469 | 15.902005462 |
| B | 4.323579151 | 10.045099531 | 13.483384865 |
| H | 4.647849233 | 11.173496944 | 13.623390640 |
| B | 3.155033699 | 7.682433798 | 14.646261266 |
| H | 2.547706682 | 7.172092806 | 15.518744601 |
| B | 4.873146009 | 7.439922089 | 12.344129380 |
| B | 5.493150791 | 8.727426034 | 13.377110021 |
| H | 6.701730368 | 8.930376291 | 13.492505127 |
| H | 5.578910664 | 6.752734994 | 11.689967492 |
| C | 0.878711595 | 7.859918047 | 13.138677793 |
| F | 0.362843356 | 7.980388392 | 11.896129774 |
| F | 0.531908888 | 6.611615515 | 13.535715973 |
| F | 0.118080154 | 8.677474975 | 13.903713821 |
| Na | 6.630000976 | 8.121830413 | 15.284302319 |

Table S21: Cartesian coordinates of complex (**3d**)

| | | | |
|---|---|---|---|
| C | 2.340332641 | 8.133774470 | 13.222367386 |
| B | 4.777774378 | 7.261624670 | 14.107802691 |
| H | 5.401539745 | 6.387843969 | 14.677074029 |
| B | 3.280848308 | 7.965550157 | 11.790042698 |
| H | 2.739882849 | 7.640192239 | 10.799644717 |
| B | 2.866991151 | 9.393906504 | 14.256109976 |
| H | 2.072975090 | 9.996863610 | 14.876817383 |
| B | 3.404308044 | 6.803067189 | 13.114565168 |
| H | 2.957089997 | 5.723023365 | 12.995529721 |
| B | 2.932688179 | 9.564838537 | 12.495975675 |
| H | 2.163973443 | 10.278199358 | 11.965154473 |
| B | 4.558067873 | 9.164052779 | 11.938977755 |
| H | 5.050771708 | 9.679512103 | 11.002452459 |
| B | 4.444463862 | 8.870066979 | 14.812992086 |
| H | 4.813404997 | 9.216401719 | 15.917708706 |
| B | 4.325186931 | 10.044020521 | 13.489204482 |
| H | 4.645023056 | 11.172637530 | 13.625831444 |
| B | 3.157824067 | 7.681517059 | 14.649024717 |
| H | 2.551073748 | 7.171211069 | 15.520096303 |
| B | 4.875251634 | 7.437987846 | 12.348716177 |
| B | 5.494973009 | 8.728362620 | 13.376304280 |
| H | 6.688054715 | 8.981196231 | 13.370740378 |
| H | 5.576187920 | 6.752008491 | 11.690585168 |
| C | 0.873331842 | 7.860064220 | 13.136004665 |
| F | 0.367171483 | 7.973924636 | 11.889688402 |
| F | 0.527323803 | 6.615635673 | 13.539487613 |
| F | 0.113672544 | 8.684366312 | 13.891744894 |
| Mg | 6.848459406 | 8.091882010 | 15.452566358 |

Table S22: Cartesian coordinates of complex (**4d**)

| | | | |
|---|---|---|---|
| C | 2.340332641 | 8.133774470 | 13.222367386 |
| B | 4.777774378 | 7.261624670 | 14.107802691 |
| H | 5.401539745 | 6.387843969 | 14.677074029 |
| B | 3.280848308 | 7.965550157 | 11.790042698 |
| H | 2.739882849 | 7.640192239 | 10.799644717 |
| B | 2.866991151 | 9.393906504 | 14.256109976 |
| H | 2.072975090 | 9.996863610 | 14.876817383 |
| B | 3.404308044 | 6.803067189 | 13.114565168 |
| H | 2.957089997 | 5.723023365 | 12.995529721 |
| B | 2.932688179 | 9.564838537 | 12.495975675 |
| H | 2.163973443 | 10.278199358 | 11.965154473 |
| B | 4.558067873 | 9.164052779 | 11.938977755 |
| H | 5.050771708 | 9.679512103 | 11.002452459 |
| B | 4.444463862 | 8.870066979 | 14.812992086 |
| H | 4.813404997 | 9.216401719 | 15.917708706 |
| B | 4.325186931 | 10.044020521 | 13.489204482 |
| H | 4.645023056 | 11.172637530 | 13.625831444 |
| B | 3.157824067 | 7.681517059 | 14.649024717 |
| H | 2.551073748 | 7.171211069 | 15.520096303 |
| B | 4.875251634 | 7.437987846 | 12.348716177 |
| B | 5.494973009 | 8.728362620 | 13.376304280 |
| H | 6.688054715 | 8.981196231 | 13.370740378 |
| H | 5.576187920 | 6.752008491 | 11.690585168 |
| C | 0.873331842 | 7.860064220 | 13.136004665 |
| F | 0.367171483 | 7.973924636 | 11.889688402 |
| F | 0.527323803 | 6.615635673 | 13.539487613 |
| F | 0.113672544 | 8.684366312 | 13.891744894 |
| Mg | 6.848459406 | 8.091882010 | 15.452566358 |