Natural indices for the chemical hardness / softness of metal cations and ligands

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Table S1  Ionic radii, solvation energies, Gibbs free energy of formation of divalent cations, and stability constants for $M^{2+}$—humic acid and $M^{2+}$—fulvic acid complexes.

| $M^{2+}$ | $r_{M^{2+}}$ (Å) | $\Delta G_{s}^{M^{2+}}$ (Exp.) | $\Delta G_{f}^{M^{2+}}$ (Exp.) | $\log K_{ML}$ | Humic acid (Exp.) | Humic acid (Calc. ± 0.37) | Fulvic acid (Exp.) | Fulvic acid (Calc. ±0.40) | ATP (Exp.) | ATP (Calc. ±0.28) | H-ATP (Exp.) | H-ATP (Calc. ±0.18) |
|----------|------------------|-----------------------------|--------------------------|------------|------------------|----------------------|-----------------------|------------------------|------------|-----------------|--------------|-------------------|
| Pt       | 0.80             | -141.87                     | 54.80                    | 8.53       | 4.38             | 5.73                 | 3.83                  |                        |            |                 |              |                   |
| Pd       | 0.80             | -141.87                     | 42.49                    | 8.27       | 4.26             | 5.58                 | 3.91                  |                        |            |                 |              |                   |
| Hg       | 1.02             | -119.71                     | 39.36                    | 8.25       | 4.46             | 3.66                 | 4.90                  |                        |            |                 |              |                   |
|          | 0.73             | -144.83                     | 15.55                    | 6.41       | 4.70             | 4.26                 | 6.13                  |                        |            |                 | 6.0           |                   |
| Cu       | 1.18             | -107.89                     | -5.79                    | 8.70       | 3.60             | 3.84                 | 5.59                  |                        |            |                 |              |                   |
| Pb       | 1.11             | -112.91                     | -6.63                    | 8.02       | 3.93             | 5.22                 | 4.02                  |                        |            |                 |              |                   |
| Sn       | 0.70             | -147.75                     | -10.90                   | 5.78       | 4.50             | 3.98                 | 5.02                  |                        |            |                 | 5.14         | 4.23              |
| Ni       | 0.74             | -144.35                     | -13.00                   | 5.20       | 4.30             | 3.99                 | 4.63                  |                        |            |                 | 5.17         | 4.19              |
| Co       | 0.95             | -125.31                     | -18.57                   | 6.90       | 3.95             | 3.54                 | 3.61                  |                        |            |                 | 5.04         | 4.92              |
| Cd       | 0.77             | -141.04                     | -21.87                   | 6.57       | 3.92             | 5.21                 | 4.10                  |                        |            |                 |              |                   |
| Fe       | 0.75             | -143.30                     | -35.17                   | 5.73       | 3.20             | 3.79                 | 4.34                  |                        |            |                 |              |                   |
| Zn       | 0.82             | -136.46                     | -55.20                   | 5.00       | 3.95             | 3.62                 | 4.77                  |                        |            |                 | 3.76         | 4.69              |
| Mn       | 0.45             | -175.02                     | -89.80                   | 4.79       | 2.70             | 2.30                 | 4.74                  |                        |            |                 | 4.63         | 4.55              |
| Be       | 0.72             | -145.80                     | -108.83                  | 4.10       | 2.70             | 2.30                 | 4.76                  |                        |            |                 | 4.72         | 4.14              |
| Mg       | 1.17             | -108.59                     | -129.10                  | 6.01       | 3.29             | 3.29                 | 5.09                  |                        |            |                 | 5.19         |                   |
| Eu       | 1.00             | -112.28                     | -132.12                  | 4.22       | 3.60             | 2.82                 | 4.85                  |                        |            |                 | 4.91         | 4.35              |
| Ca       | 1.36             | -95.99                      | -132.73                  | 8.03       | 2.29             | 5.28                 | 4.03                  |                        |            |                 |              |                   |
| Ba       | 1.16             | -109.30                     | -133.72                  | 5.82       | 2.63             | 5.10                 | 4.08                  |                        |            |                 |              |                   |
| Sr       | 1.39             | -94.14                      | -134.20                  | 8.37       | 2.21             | 3.21                 | 5.25                  |                        |            |                 |              |                   |
| Ra       | 0.75             | -142.54                     | -227.70                  | 1.37       | 1.92             | 2.47                 | 5.45                  |                        |            |                 |              |                   |

ATP = Adenosine-5’-triphosphate; H-ATP = protonated ATP that forms metal complexes in M-HL form.
Note: Radii of the cations are from references of\textsuperscript{15}. The values of log K metal—complexes for ATP and H-ATP in ionic strength of 0.1 are from reference\textsuperscript{17}. M—humates data are from\textsuperscript{20} and\textsuperscript{33}. Cu(II)—humate is not used because it is pH-dependent and related to the formation of polynuclear complexes (i.e., both ML and ML\textsubscript{2} complexes)\textsuperscript{34}. The data for M—fulvic acid complexes are from Schnitzer and colleagues\textsuperscript{35-37}. There are two reported values for Cu—fulvic acid complex. The values of ΔG\textsubscript{f} of the cations are from references\textsuperscript{12,16,18}, except for Pt\textsuperscript{2+}, Pd\textsuperscript{2+} from reference\textsuperscript{24}.

![Figure S1: Plots showing experimental values vs. calculated values for M—ATP (left) and M—H-ATP (right) complexes.](image-url)