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)	ΔG_s $M^{2+}_{(aq)}$	ΔG_f $M^{2+}_{(aq)}$	*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
Cu	0.73	-144.83	15.55		6.41	4.70	4.26	6.13; **6.0**	5.52	3.52	3.86
Pb	1.18	-107.89	-5.79	8.70	8.68	3.60	3.84		5.59		3.67
Sn	1.11	-112.91	-6.63		8.02		3.93		5.22		4.02
Ni	0.70	-147.75	-10.90	5.78	5.82	4.50	3.98	5.02	5.14	4.23	4.06
Co	0.74	-144.35	-13.00	5.20	5.82	4.30	3.99	4.63	5.17	4.19	4.05
Cd	0.95	-125.31	-18.57	6.90	6.57		3.95	3.54	3.61	5.04	4.92
Fe	0.77	-141.04	-21.87		5.71		3.92		5.21		4.10
Zn	0.75	-143.30	-35.17	5.73	5.35	3.20	3.79		3.49		5.04
Mn	0.82	-136.46	-55.20	5.00	5.17	3.95	3.62	3.77	3.76	4.69	4.79
Be	0.45	-175.02	-89.80		4.79		2.79	4.06	3.93	4.55	4.69
Mg	0.72	-145.80	-108.83	4.10	3.80	2.70	2.30	4.76	4.72	4.14	4.27
Eu	1.17	-108.59	-129.10		6.01		2.66	3.29	3.29	5.09	5.19
Ca	1.00	-121.28	-132.12	4.22	4.20	3.60	2.82	4.85	4.91	4.35	4.18
Ba	1.36	-95.99	-132.73		8.03		2.29		5.28		4.03
Sr	1.16	-109.30	-133.72		5.82		2.63		5.10		4.08
Ra	1.39	-94.14	-134.20		8.37		2.21		3.21		5.25
UO_2	0.75	-142.54	-227.70		1.37		1.92		2.47		5.45

ATP = Adenosine-5'-tiphosphate; H-ATP = protonated ATP that forms metal complexes in M-HL form.

Note: Radii of the cations are from references of [15]. The values of *log* K metal—complexes for ATP and H-ATP in ionic strength of 0.1 are from reference [17]. M—humates data are from [20] and [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_2 complexes) [34]. The data for M—fulvic acid complexes are from Schnitzer and colleagues [35-37]. There are two reported values for Cu-fulvic acid complex. The values of ΔG_f of the cations are from references [12, 16, 18], except for Pt^{2+}, Pd^{2+} from reference [24].

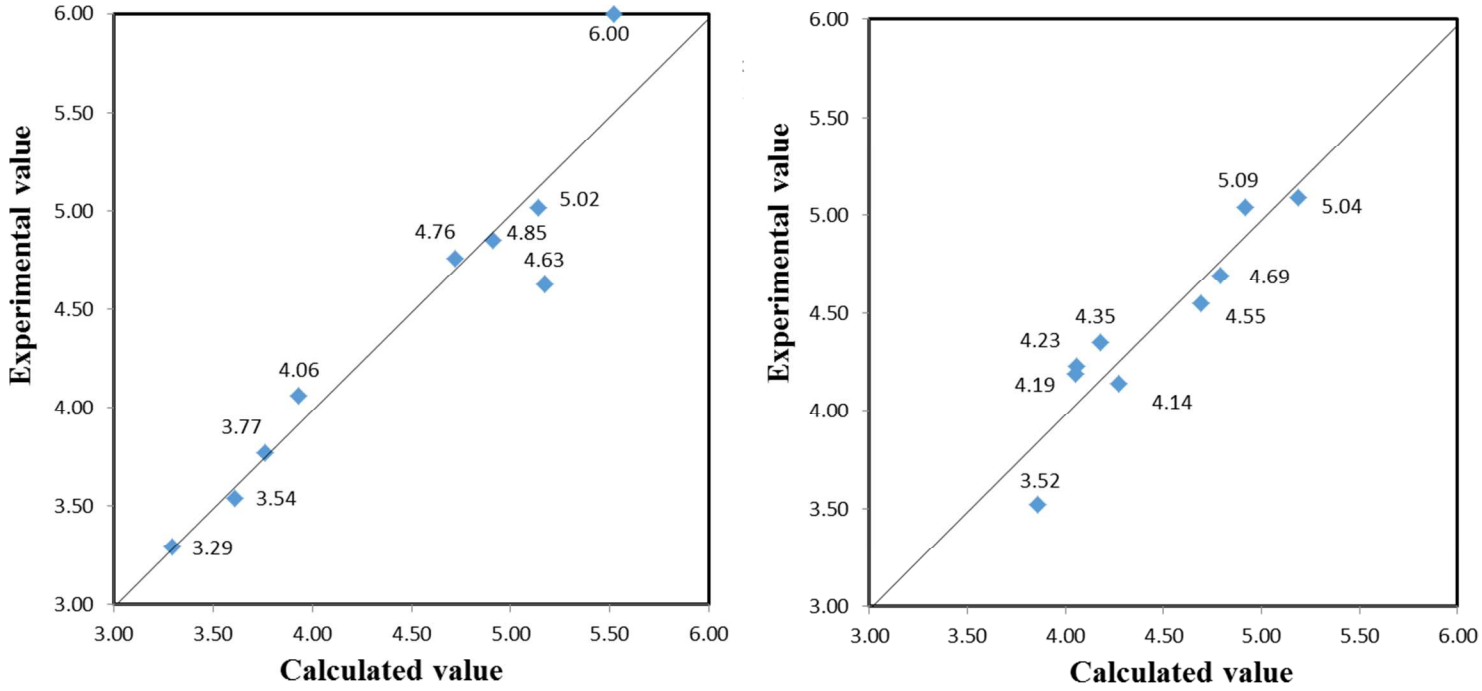

Figure S1: Plots showing experimental values vs. calculated values for M—ATP (left) and M—H-ATP (right) complexes.