Electronic Supplementary Material (ESI) for Dalton Transactions

Interaction of d^{10} Metal Ions with thioether ligands: a thermodynamic and theoretical study.

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Electronic Supplementary Material

Table S1 Experimental and calculated M-S bond distances for the $[M(9AneS3)_2]^{2+}$ complexes. Also the weighted RMS obtained when superimposing (using gOpenMol graphics program) the calculated and experimental structures of the $[M(9AneS3)_2]^{2+}$ complexes is reported. All functionals were used employing the same basis set (SDD ECP for the metal ion and 6-311++G(d,p)) .

CSD code	Ref.	metal	M-$S_{exp.}$ (Å)	M-$S_{calc.}$ (Å)			Weighted RMS		
				PBE	B3LYP	M06	PBE	B3LYP	M06
VEJNON	40	Zn	2.496	2.528	2.575	2.530	0.0212	0.0467	0.0244
AQADIF	36	Cd	2.658	2.705	2.753	2.707	0.0277	0.0538	0.0309
EZILEE	65	Hg	2.683	2.750	2.810	2.770	0.0482	0.0789	0.0544
FIJTOH10	44	Ag	2.725	2.754	2.821	2.761	0.0098	0.061	0.050

Table S2 Calculated ΔH values (kJ mol^{-1}) relative to the reactions in Figure S2

	$\Delta H_{1,gas}$	$\Delta H_{2,gas}$
Zn^{2+}	-1194.1	-408.4
Cd^{2+}	-970.3	-399.2
Hg^{2+}	-1111.3	-378.2
Ag^{+}	-359.4	-158.2

Table S3 Calculated ΔH and ΔG values (kJ mol^{-1}) for the reactions 5 and 6 (Figures 6 and 7, in the article)

	Gas phase with coordinated AN				*AN (PCM)*			
	ΔH(5)	ΔH(6)	ΔG(5)	ΔG(6)	ΔH(5)	ΔH(6)	ΔG(5)	ΔG(6)
Zn^{2+}	56.9	54.4	-11.4	-1.3	-14.7	-18.2	-37.2	-28.2
Cd^{2+}	58.6	56.1	-9.7	4.2	-14.8	-36.8	-37.2	-42.8
Hg^{2+}	8.4	8.8	-57.1	-40.8	-72.6	-83.4	-92.6	-87.2
Ag^{+}	8.4	-47.3	-30.4	-41.1	-49.2	-17.8	-42.1	-11.4

Figure S1 Experimental *vs.* theoretical free energies of solvation in acetonitrile (ΔG_{sv}) for the three cations studied in this work.

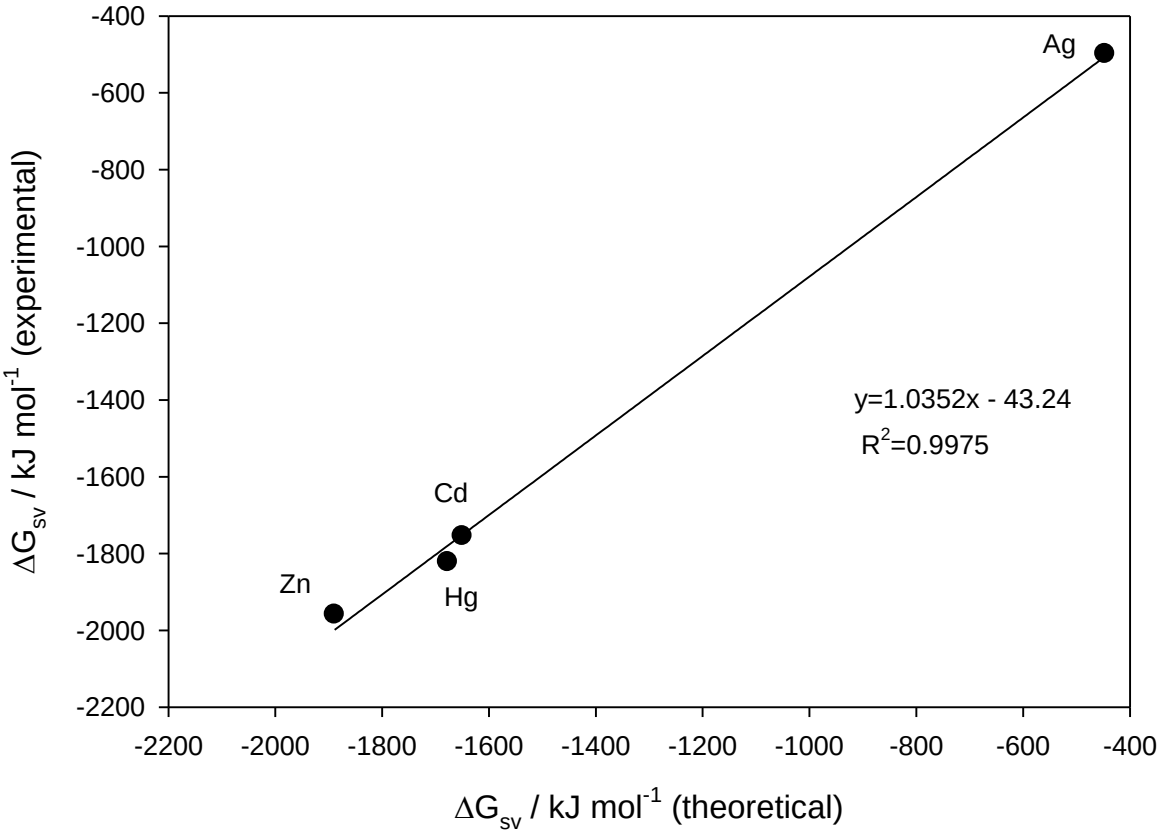

Figure S2 Calculated reaction enthalpy values, ΔH_{1gas} and ΔH_{2gas}, for the reactions: $M^{n+}_{(g)} + 9AneS3_{(g)} \rightarrow [M(9AneS3)]^{n+}_{(g)}$ (red) and $[M(9AneS3)]^{n+}_{(g)} + 9AneS3_{(g)} \rightarrow [M(9AneS3)]^{n+}_{2\ (g)}$ (light blue) respectively, in gas phase.