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CORRECTION

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Correction: Structural characterization of gas-phase cysteine and cysteine methyl ester complexes with zinc and cadmium dications by infrared multiple photon dissociation spectroscopy

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Correction for 'Structural characterization of gas-phase cysteine and cysteine methyl ester complexes with zinc and cadmium dications by infrared multiple photon dissociation spectroscopy' by Rebecca A. Coates *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 25799–25808.

Although the overall conclusions of the original article remain unaffected (no experimental or theoretical IR spectra are changed, nor is any calculated thermochemistry at 0 K), the thermal corrections to the Gibbs free energy at 298 K were mistakenly overestimated. Corrected 298 K values for Tables 1 and 2 from the original manuscript are given below. Notably, only very subtle changes are found such that the relative order of all 298 K theoretically determined low-energy species remains the same for the $[\mathrm{Zn(Cys\text{-}H)}]^+$, $[\mathrm{Cd(Cys\text{-}H)}]^+$, $[\mathrm{Zn(CysOMe\text{-}H)}]^+$, $[\mathrm{Cd(CysOMe\text{-}H)}]^+$ and $\mathrm{CdCl^+(CysOMe)}$ systems. Therefore, we have not corrected the relative energies used throughout the text.

Table 1 B3LYP,[a] B3P86, and MP2(full) relative free energies (kJ mol^{-1}) at 298 K of low-lying conformers of $[\mathrm{M(Cys\text{-}H)}]^+$ and $[\mathrm{M(CysOMe\text{-}H)}]^{+b}$

Complex	Structure	Zn	Cd
$[\mathrm{M(Cys\text{-}H)}]^+$	[N,CO,S$^-$]*tgg*	0.0 (0.0), 0.0, 0.0	0.0 (0.0), 0.0, 0.0
	[N,CO,S$^-$]*cgg*	24.4 (24.0), 24.0, 23.2	25.1 (24.9), 24.7, 25.9
	[CO,S$^-$]*cgg*	27.8 (32.8), 31.5, 45.0	23.1 (28.5), 28.1, 33.0
	[N,S$^-$]*tgt*	30.8 (35.1), 37.7, 38.0	27.7 (34.0), 29.8, 44.0
	[CO$^-$,S$^-$]*cgg*[c]	36.0 (36.9), 40.5, 42.0	30.5 (29.4), 34.9, 30.9
	[N,OH,S$^-$]*tgg*	38.2 (36.3), 42.1, 35.2	41.7 (46.0), 44.4, 58.0
	[CO,S$^-$]*ctg*	50.2 (54.0), 54.6, 68.5	44.8 (46.2), 46.1, 49.9
	[N,CO$^-$,S]*ggg*	60.6 (57.7), 60.9, 58.2	55.9 (60.2), 60.0, 65.7
	[N,S$^-$]*cgt*	63.9 (67.2), 70.2, 71.5	77.0 (86.0), 91.5, 98.7
	[N$^-$,CO,S]*tggg*	100.5 (101.2), 101.5, 102.8	104.5 (108.8), 106.6, 112.6
	[S$^-$]*tgg*	143.8 (150.7), 164.3, 179.9	86.3 (95.2), 100.7, 107.9
$[\mathrm{M(CysOMe\text{-}H)}]^+$	[N,CO,S$^-$]*tgg*	0.0 (0.0), 0.0, 0.0	0.0 (0.0), 0.0, 0.0
	[N,CO,S$^-$]*cgg*	36.2 (33.4), 35.2, 36.2	37.2 (34.6), 36.0, 37.6
	[N,OMe,S$^-$]*tgg*	43.7 (38.9), 46.3, 37.2	36.7 (32.8), 39.5, 33.2
	[N,S$^-$]*tgt*	36.9 (41.2), 43.4, 46.5	27.0 (32.4), 31.5, 37.2
	[CO,S$^-$]*tgg*	55.5 (61.2), 64.0, 74.1	50.7 (57.4), 57.3, 70.0
	[CO,S$^-$]*ctg*	76.9 (77.6), 83.5, 93.6	72.3 (74.2), 77.0, 90.6
	[N,S$^-$]*cgt*	84.3 (84.7), 89.5, 92.8	73.1 (74.5), 76.3, 82.1
	[N$^-$,CO,S]*tggg*	102.3 (102.6), 103.3, 105.9	104.4 (104.6), 106.4, 112.7

[a] Values including empirical dispersion corrections are given in parentheses. [b] Calculations performed at the B3LYP, B3P86, and MP2(full) levels of theory using a 6-311+G(2d,2p) basis set for Zn-containing complexes and def2TZVPP for Cd-containing complexes. Geometries and vibrational frequencies calculated at the B3LYP/6-311+G(d,p) level for Zn-containing complexes and B3LYP/def2TZVP for Cd-containing complexes. [c] Salt bridge between $\mathrm{NH3^+}$, $\mathrm{CO_2^-}$, and $\mathrm{S^-}$ groups.

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Table 2 Relative free energies (kJ mol^{-1}) at 298 K of low-lying CdCl$^+$(CysOMe) conformers[a]

Structure	B3LYP[b]	B3P86	MP2(full)
[N,CO,S]$tggg_+$	0.0 (0.0)	0.0	0.0
[N,CO,S]$tggg_-$	1.1 (1.7)	1.2	1.7
[S$^-$]*tcg*[c]	17.6 (19.0)	18.2	21.5
[N,CO]$tgtg_-$	20.1 (29.3)	24.9	31.1
[N,CO]*tggg*	20.7 (29.2)	25.3	30.7
[N,CO]*tcgg*	21.2 (30.2)	25.9	31.8
[N,S]*tgtg*	23.4 (30.3)	26.0	33.7
[N,CO]$tgtg_+$	23.4 (32.8)	28.3	35.0
[CO,S$^-$]*ttg*[c]	26.0 (30.1)	26.7	31.0
[N,OMe,S]$tggg_+$	27.7 (22.2)	28.6	21.5
[N,OMe,S]$tggg_-$	32.2 (27.7)	33.4	26.7
[N,CO,S]*cggg*	38.8 (36.1)	37.9	39.2
[CO,S]*ttgt*	51.0 (58.8)	56.8	72.6
[CO,S$^-$]*cgg*[c]	66.2 (66.8)	64.7	72.2
[CO,S]*ctgt*	82.5 (88.9)	87.6	104.2

[a] Calculations performed at the stated level of theory using a def2TZVPP basis set. Geometries and vibrational frequencies calculated at the B3LYP/def2TZVP level of theory. [b] Values including empirical dispersion corrections are given in parentheses. [c] Salt bridge between NH3$^+$, CO_2^-, and S$^-$ groups.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.