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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 [Zn(Cys-H)]⁺, [Cd(Cys-H)]⁺, [Zn(CysOMe-H)]⁺, [Cd(CysOMe-H)]⁺ and 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 [M(Cys-H)]⁺ and [M(CysOMe-H)]⁺^b

| Complex | Structure | Zn | Cd |
|----------------------------|--|-----------------------------|-----------------------------|
| [M(Cys-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]lggg | 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 |
| [M(CysOMe-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/def2TZVPP for Cd-containing complexes. ^c Salt bridge between NH₃⁺, CO₂⁻, and 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⁺, CO₂⁻, and S⁻ groups.

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

