PCCP



CORRECTION

View Article Online



Cite this: Phys. Chem. Chem. Phys., 2017, 19, 18777

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

Rebecca A. Coates, a Christopher P. McNary, a Georgia C. Boles, a Giel Berden, b Jos Oomensbc and P. B. Armentrout 10 *a

DOI: 10.1039/c7cp90144e

rsc.li/pccp

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, 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)]⁺

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]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
[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/def2TZVP for Cd-containing complexes. ^c Salt bridge between NH3⁺, CO₂⁻, and S⁻ groups.

^a Department of Chemistry, University of Utah, Salt Lake City, UT 84112, USA. E-mail: armentrout@chem.utah.edu

^b Radboud University, Institute for Molecules and Materials, FELIX Laboratory, Toernooiveld 7, NL-6525ED Nijmegen, The Netherlands

^cvan't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands

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

Structure	$\mathrm{B3LYP}^b$	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.