

Cite this: *Dalton Trans.*, 2019, **48**, 12755

Correction: Substituents drive ligand rearrangements, giving dinuclear rather than mononuclear complexes, and tune Co^{II/III} redox potential†

Fabrice N. H. Karabulut, Humphrey L. C. Feltham and Sally Brooker*

DOI: 10.1039/c9dt90173f
rsc.li/daltonCorrection for 'Substituents drive ligand rearrangements, giving dinuclear rather than mononuclear complexes, and tune Co^{II/III} redox potential' by Fabrice N. H. Karabulut *et al.*, *Dalton Trans.*, 2018, **47**, 11749–11759, DOI: 10.1039/c8dt01502c.

Unfortunately many corrections need to be made to both the manuscript and ESI file. For optimal clarity, the key points are summarised in the bullet points below, with more details provided below that (and for the corrected ESI tables and figures please see the corrected ESI file, republished 29th July 2019).

1. There were numerous errors in the reporting of the elemental analysis and TGA data for this paper (resulting in a revised solvent content for the bulk samples), and missed recrystallisation steps in the experimental section (after which yields are lower than reported initially). Samples of all complexes were re-prepared in the course of putting these corrections together – the revised solvent content and yield of each of the samples is detailed below.

2. Due to point 1, everywhere in the paper and ESI file when we referred to 2·2H₂O and 3·3.5H₂O should now read [Co^{II}(L^{BrH-OBF₃})₂](BF₄)₂·4H₂O (2') and [Co^{II}(L^{ClH-OBF₃})₂](BF₄)₂·2H₂O (3'). Methanolysis of 2' and 3' presumably occurs to give the single crystals of 2-solvents and 3-solvents, the structures of which are correctly reported in the paper.

3. The PF₆ complexes are only a very minor component of this paper (sentence in abstract p. 11749; synthesis discussion paragraph p. 11752; sentence in conclusion p. 11755; experimental sections starting at bottom p. 11756 and finishing p. 11757) but repeating these syntheses proved non-trivial so please disregard any comments made about those complexes, as they have never been made in analytically pure form.

Experimental

HL^{HBr}. Elemental analysis: C 42.25, H 3.23, N 13.10, Calc. for [C₁₅H₁₄N₄OBr₂] (426.1 g mol⁻¹): C 42.28, H 3.31, N 13.15.

HL^{BrH}. Elemental analysis: C 42.20, H 3.10, N 12.95, Calc. for [C₁₅H₁₄N₄OBr₂] (426.1 g mol⁻¹): C 42.28, H 3.31, N 13.15.

HL^{ClH}. Elemental analysis: C 51.82, H 4.05, N 16.30, Calc. for [C₁₅H₁₄N₄OCl₂]·0.5H₂O (346.2 g mol⁻¹): C 52.04, H 4.37, N 16.18.

[Co^{II}(HL^{HBr})(H₂O)₂](BF₄)₂ (1'). (35 mg, 28%). Elemental analysis: C 25.77, H 2.50, N 7.82, Calc. for 1' (694.7 g mol⁻¹): C 25.93, H 2.61, N 8.07. TGA (5.026 mg, 80 °C for 180 min) found 5.48%; calculated weight loss for removal of 2H₂O: 5.18%.

[Co^{II}(L^{BrH-OBF₃})₂](BF₄)₂·4H₂O (2'). In air, solid HL^{BrH} (53.5 mg, 0.126 mmol) was added to a pink solution of Co(BF₄)₂·6H₂O (43 mg, 0.126 mmol) in MeOH (20 mL). The red solution was stirred for 6 hours, concentrated to 5 mL under reduced pressure and finally subjected to diethyl ether vapour diffusion. The resulting red powder was filtered off, air dried and subjected a second time to diethyl ether vapour diffusion into MeOH, to give [Co^{II}(L^{BrH-OBF₃})₂](BF₄)₂·4H₂O (11 mg, 7%). Elemental analysis: C 27.06, H 2.69, N 8.68, Calc. for 2' (tetrahydrate: 1349.3 g mol⁻¹): C 26.70, H 2.54, N 8.30. TGA (3.353 mg, 80 °C for 60 min)

Department of Chemistry and MacDiarmid Institute of Advanced Materials and Nanotechnology, University of Otago, PO Box 56, Dunedin 9054, New Zealand.

E-mail: sbrooker@chemistry.otago.ac.nz

† Electronic supplementary information (ESI) available: Additional CSD search results; NMR spectra; possible ligand tautomers; IR spectra; microanalysis/TGA comparisons; X-ray crystallography tables; cyclic voltammetry results. CCDC reference numbers 1837189–1837191. For ESI and crystallographic data in CIF or other electronic format see DOI: 10.1039/c9dt90173f



found 5.74%; calculated weight loss for removal of 4H₂O: 5.34%. Some single crystals of [Co^{II}(L^{BrH-BF₂OMe})₂](BF₄)₂·solvents (2·solvents) formed on recrystallisation of 2' from MeOH/Et₂O (methanolysis presumably converts ligand-O-BF₃ to ligand-O-BF₂OMe).

[Co^{II}(L^{ClH-OBF₃})₂](BF₄)₂·2H₂O (3'). In air, solid HL^{ClH} (59 mg, 0.175 mmol) was added to a pink solution of Co(BF₄)₂·6H₂O (59.6 mg, 0.175 mmol) in MeOH (20 mL). The red solution was stirred for 6 hours, concentrated to 5 mL under reduced pressure and finally subjected to diethyl ether vapour diffusion. The resulting red powder was filtered off, air dried and subjected a second time to diethyl ether vapour diffusion into MeOH, to give [Co^{II}(L^{ClH-OBF₃})₂](BF₄)₂·2H₂O (16 mg, 8%). Elemental analysis: C 31.49, H 3.09, N 10.29, Calc. for 3' (dihydrate: 1135.5 g mol⁻¹): C 31.73, H 2.66, N 9.87. TGA (3.226 mg, 80 °C for 180 min) found 2.96%; calculated weight loss for removal of 2H₂O: 3.17%. Single crystals of [Co^{II}(L^{ClH-BF₂OMe})₂](BF₄)₂·solvents (3·solvents) formed on recrystallisation of 3' from MeOH/Et₂O (methanolysis presumably converts ligand-O-BF₃ to ligand-O-BF₂OMe).

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

