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Correction: When SF₅ outplays CF₃: effects of pentafluorosulfanyl decorated scorpionates on copper

Anurag Noonikara-Poyil,^a Alvaro Muñoz-Castro,^b Andrii Boretskyi,^c
Pavel K. Mykhailiuk^{*de} and H. V. Rasika Dias^{*a}

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Correction for 'When SF₅ outplays CF₃: effects of pentafluorosulfanyl decorated scorpionates on copper' by Anurag Noonikara-Poyil *et al.*, *Chem. Sci.*, 2021, 12, 14618–14623, <https://doi.org/10.1039/D1SC04846E>.

The authors regret that in the original version of the manuscript, an inadvertent error was made during percent buried volume calculation and topographical steric map creation of bis(pyrazolyl)borate supporting ligands of [Ph₂B(3-(SF₅)Pz)₂]Cu(C₂H₄), [Ph₂B(3-(CF₃)Pz)₂]Cu(C₂H₄), [Ph₂B(3-(SF₅)Pz)₂]Cu(CO) and [Ph₂B(3-(CF₃)Pz)₂]Cu(CO) using SambVca. This was caused due to the removal of only ethylene and CO groups, rather than the entire Cu–ethylene or Cu–CO moiety (including the metal atom) as suggested by SambVca protocol. Correct percent buried volumes (%V_{bur}) pertinent to the results and discussion section are given below.

Compound	%V _{bur}
[Ph ₂ B(3-(SF ₅)Pz) ₂]Cu(C ₂ H ₄)	65.6
[Ph ₂ B(3-(CF ₃)Pz) ₂]Cu(C ₂ H ₄)	59.5
[Ph ₂ B(3-(SF ₅)Pz) ₂]Cu(CO)	68.7
[Ph ₂ B(3-(CF ₃)Pz) ₂]Cu(CO)	60.8

The corrected versions of Fig. 3, S40 and S41 can be found below. The electronic supplementary information (ESI) available online has now been updated to reflect these changes.

^aDepartment of Chemistry and Biochemistry, The University of Texas at Arlington, Arlington, TX 76019, USA. E-mail: dias@uta.edu^bGrupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingeniería, Universidad Autónoma de Chile, El Llano Subercaseaux 2801, Santiago, Chile^cUORSY, Ukrorgsintez Ltd, PO Box 59, 02002 Kyiv, Ukraine^dEnamine Ltd, Chervonotkatska 78, 02094, Kyiv, Ukraine^eChemistry Department, Taras Shevchenko National University of Kyiv, Volodymyrska 64, 01601 Kyiv, Ukraine. E-mail: Pavel.Mykhailiuk@gmail.com

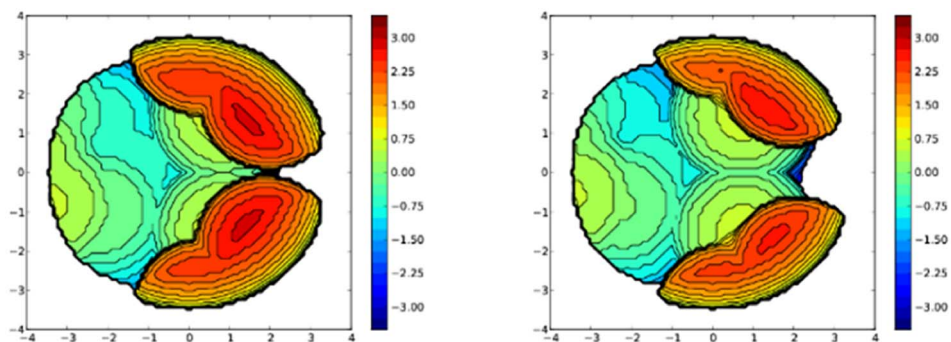
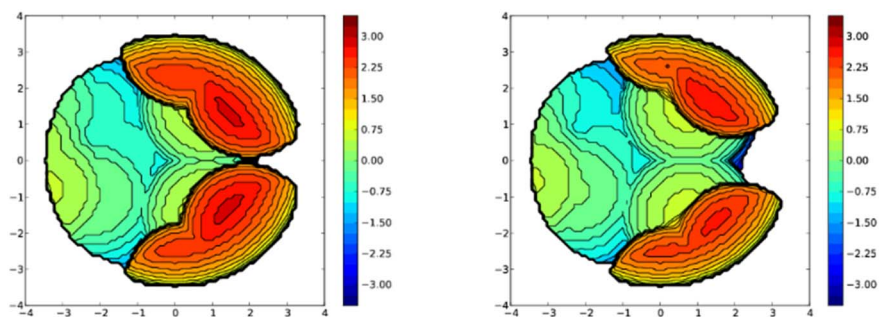


Fig. 3 Steric maps of bis(pyrazolyl)borate ligands in $[\text{Ph}_2\text{B}(3\text{-(SF}_5\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$ (left) and $[\text{Ph}_2\text{B}(3\text{-(CF}_3\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$ (right). The related % buried volume ($\%V_{\text{bur}}$) values are 65.6 (average for the two molecules in the asymmetric unit) and 59.5, respectively.



$[\text{Ph}_2\text{B}(3\text{-(SF}_5\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$

$[\text{Ph}_2\text{B}(3\text{-(CF}_3\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$

Fig. S40 Steric maps of bis(pyrazolyl)borate ligands in $[\text{Ph}_2\text{B}(3\text{-(SF}_5\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$ (left) and $[\text{Ph}_2\text{B}(3\text{-(CF}_3\text{)Pz})_2]\text{Cu}(\text{C}_2\text{H}_4)$ (right) based on X-ray data. The resulting % buried volume ($\%V_{\text{bur}}$) values are 65.6 (average of 66.1 and 65.0 for the two molecules in the asymmetric unit) and 59.5, respectively.



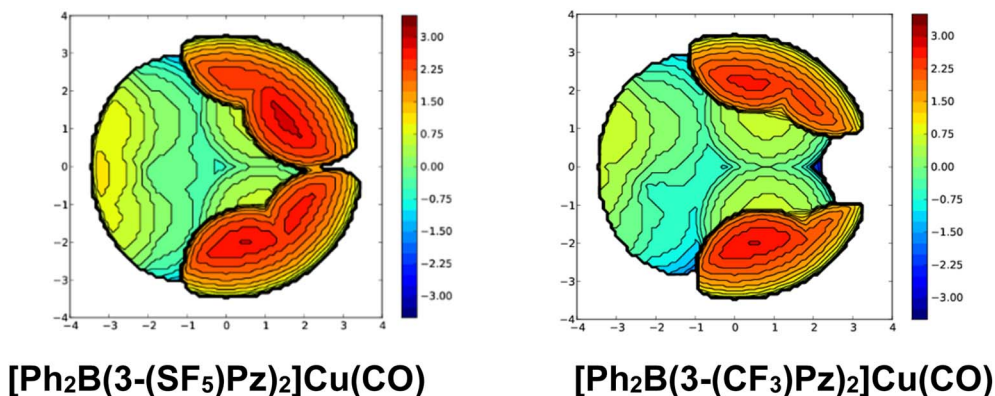


Fig. S41 Steric maps of bis(pyrazolyl)borate ligands in [Ph₂B(3-(SF₅)Pz)₂]Cu(CO) (left) and [Ph₂B(3-(CF₃)Pz)₂]Cu(CO) (right) based on X-ray data. The resulting % buried volume (%V_{bur}) values are 68.7 (average of 69.0 and 68.4 for the two molecules in the asymmetric unit) and 60.8 (fluorine atoms of one of the CF₃ groups of [Ph₂B(3-(CF₃)Pz)₂]Cu(CO) show positional disorder, and only the major occupancy fluorine atoms were utilized in the calculation to avoid inflated steric bulk), respectively. For comparison, inclusion of both disorder-parts in [Ph₂B(3-(CF₃)Pz)₂]Cu(CO) leads to a marginally higher %V_{bur} value of 61.9.

The percent buried volumes (%V_{bur}) and the steric maps were computed using SambVca 2.1 (<https://www.aocdweb.com/OMtools/sambvca2.1/>) for a sphere radius of 3.5 Å about the metal center, Bondi van der Waals radii scaled by a factor of 1.17, 0.10 Å mesh spacing, and including hydrogen atoms. The %V_{bur} values for [Ph₂B(3-(SF₅)Pz)₂]Cu(C₂H₄) and [Ph₂B(3-(SF₅)Pz)₂]Cu(CO) are the average of two molecules of each type in the asymmetric unit.

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

