



Cite this: *Chem. Commun.*, 2018, 54, 12271

DOI: 10.1039/c8cc90442a

rsc.li/chemcomm

Correction: Synthesis of $\text{Ca}(\text{PF}_6)_2$, formed via nitrosonium oxidation of calcium

Evan N. Keyzer,^a Peter D. Matthews,^{ab} Zigeng Liu,^a Andrew D. Bond,^a Clare P. Grey^{*a} and Dominic S. Wright^{*a}

Correction for 'Synthesis of $\text{Ca}(\text{PF}_6)_2$, formed via nitrosonium oxidation of calcium' by Evan N. Keyzer *et al.*, *Chem. Commun.*, 2017, **53**, 4573–4576.

In the original article, Fig. 2 shows the structure of a $\text{Ca}(\text{PF}_6)_2$ species. Upon further analysis, the authors discovered that the structure is in fact $[(\text{Ca} \subset 15\text{-crown-5})_4(\text{SiF}_6)_2(\text{CH}_3\text{CN})_2]^{4+}(\text{PF}_6^-)_4$, with bridging SiF_6^{2-} ligands rather than bridging PF_6^- . It appears that this error arose simply from picking a minor decomposition product during X-ray analysis as SiF_6^{2-} was not observed in the ^{19}F NMR spectrum of the sample. The SiF_6^{2-} anion presumably arises from scavenging from the glass reaction vessel. The elemental analysis of this compound reported in the paper is of the mixture of products. A corrected CIF has been deposited at the CCDC (CCDC 1529827). This error does not affect the conclusion of the paper. A modified Fig. 2 is provided below, showing another example of a pure $\text{Ca}(\text{PF}_6)_2$ species (**2a**) produced using the identical procedure: $[\text{Ca} \subset (15\text{-crown-5})(\text{CH}_3\text{CN})_3]^{2+}[\text{Ca} \subset (15\text{-crown-5})_2]^{2+}(\text{PF}_6^-)_4$ (CCDC 1556067). Again, the ^{19}F and ^{31}P NMR spectra show no evidence of decomposition to PO_2F_2^- or SiF_6^{2-} . Bulk purity of this sample was confirmed by elemental analysis [anal. calcd for $\text{C}_{36}\text{H}_{69}\text{Ca}_2\text{F}_{24}\text{N}_3\text{O}_{15}\text{P}_4$ (**2a**): C, 29.95; H, 4.82; N, 2.91; P, 8.58; found: C, 28.81; H, 4.83; N, 3.01; P, 8.86].

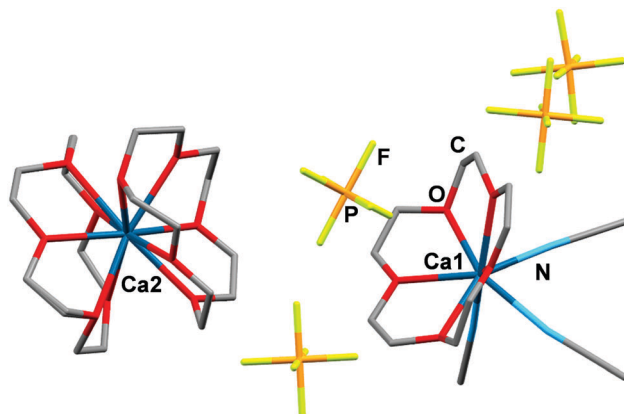


Fig. 2 Crystal structure of **2a**. Protons and disorder have been omitted for clarity (Ca, dark blue; C, grey; F, yellow; N, light blue; O, red; P, orange).

The authors apologise for these errors and any consequent inconvenience to editors and readers.

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

^a Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK. E-mail: cpg27@cam.ac.uk, dsw1000@cam.ac.uk

^b School of Chemistry, University of Manchester, Oxford Road, Manchester, M13 9BL, UK

