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Erratum: "Practical guide for curve fitting in x-ray photoelectron spectroscopy" [J. Vac. Sci. Technol. A 38, 061203 (2020)]

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The two large O 1s fit components in Fig. 4(b) in our original paper[1] (Fig. 1 here) are identified and/or labeled three times in this paper. Two of these identifications/labels are correct, and one is incorrect.

- The text is correct when it reads: "Out of the four total oxygens, half are present in the O = C part of the carboxyl/ester group (labeled 1) at 531.6 eV, and the other half are in the O-C part of the carboxyl/ester group (labeled 2) at 533.2 eV."
- Figure 4(b) also correctly labels the oxygen signals in the sense that (i) the O-C oxygen is labeled with a blue "2" and the fit component for this signal is blue, and (ii) the O = C oxygen is labeled with a green "1" and the fit component for this signal is green.
- However, the flat ends (not points) of the arrows identifying the chemical states in Fig. 4(b) are not correct. The green arrow pointing to the fit component at 531.6 eV should begin at the O = C oxygen in the chemical structure above the spectrum (as it does now in Fig. 1), and the blue arrow pointing to the fit component at 533.2 eV should begin at the O-C oxygen in the chemical structure above the spectrum (as it does now in Fig. 1). That is, the arrows in Fig. 1 here are now correct.

We take this opportunity to describe a fairly easy way to remember how to label the two O 1s signals from an ester in x-ray photoelectron spectroscopy (XPS) peak fitting. First, it is well known in organic chemistry that the resonance structures associated with the carbonyl (C = O) group, and also related functional groups containing the C = O moiety, are often consistent with and descriptive of the chemistry of these groups. However, before we proceed further, please remember that resonance structures are not real chemical structures. The real chemical structure represented by resonance structures is better described as a weighted average of the resonance structures than as any of the individual resonance structures themselves. Of course, the most accurate approach for understanding chemical structures is to perform first principles calculations on them. Resonance structures are a rapid method/tool for providing insight into chemical structures and reactivity. Figure 2 shows two resonance structures of the PET polymer shown in Fig. 4 of the original document (Fig. 1 here). In particular, Fig. 2(a) shows the original polymer as it was drawn in Fig. 4 of the original document (Fig. 1 here), and Fig. 2(b) shows a resonance structure for this molecule that was created by moving a pair of electrons on an original O-C oxygen to the O-C bond, creating another chemical bond, while simultaneously breaking one of the O-C bonds in the C = O group and adding an extra pair of electrons to the original O = C oxygen. As is customary in organic chemistry, these electron pairs are implied, not shown. The resonance structure in Fig. 2(b) now has a formal positive charge on