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The isocontour plots of Figs. 2 and 3 in the original published version of this paper1 correspond to an isocontour value of $|\Psi| = 0.010$ a.u. not 0.025 a.u. The corresponding isocontour plots at $|\Psi| = 0.025$ a.u. are shown here as Fig. 1.

Compared with the published isocontour plots at $|\Psi| = 0.010$ a.u. (Fig. 2 on p. 024719-4 and Fig. 3 on p. 024719-5), it seems that there is a little difference between the electronic structures. However, the related discussion and conclusion based on these electronic structures (the third and fourth paragraph of p. 024719-4) have not affected. In recent years, the isocontour plots are widely used at a value of $|\Psi| = 0.025$ a.u. In this case, the isocontour plots at 0.010 a.u. are better to show the wide spread of the positive charge in the cation. And the isocontour plots at 0.025 a.u. are better to show the high localization of HOMO, LUMO, and the excess electron in the anion. Therefore, the paper’s overall conclusions are unchanged.


FIG. 1. Isocontour plots of HOMO (a) and LUMO (b) and spin-density surfaces of the cation (c) and the anion (d) for the Ga2(saph)2q2 molecule obtained at the ROB3LYP/6–31G(d) level. All the MO surfaces correspond to an isocontour value of $|\Psi| = 0.025$ a.u.

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