On the Second Moments of the Electronic Charge Distributions in FClCO

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The derivation of some Zeeman parameters for FCICO is reconsidered and the corrected values are reported.

The paper by Maksić and Mikac [1] has reported a comparison of experimental and/or ab initio values of the second moments of the electronic charge distributions $\langle r_i^2 \rangle$ with those calculated by using additive formulae, for a number of molecules. In contrast to the general resulting good agreement, the large discrepancy between the experimental in plane second moments $\langle a^2 \rangle$ and $\langle b^2 \rangle$ of FClCO [2] and the calculated ones [1] suggested the possibility of the experimental quantities being in error. The case is here reconsidered and the results reported.

Since the quantities in discussion were not directly obtained from the experiment itself, but after a calculation process, as described in Ref. [2], it seemed likely that errors had occurred at this rather than at the experimental stage. In fact, by repeating the calculation procedure, it resulted that the nuclear second moments had been wrongly computed and most of the Zeeman parameters in Table 5 of [2], consequently. The corrected nuclear second moments, in units of 10^{-16} cm^2, are:

$$\sum_n Z_n a_n^2 = 46.4 \pm 1.0;$$

$$\sum_n Z_n b_n^2 = 20.9 \pm 0.5; \quad \sum_n Z_n c_n^2 = 0.0.$$

Table 1. Recalculated Zeeman parameters for FClCO. Second moments of the electronic charge anisotropies, in units of 10^{-16} cm^2, second moments of the electronic charge distributions, in units of 10^{-6} erg/(G^{-2} mole). The cgs-Gaussian units are used for consistency with the Zeeman literature. The conversion to the SI units is $(\mathrm{m}^2/\mathrm{cm}^2) \times 10^{-4}$ and $(\mathrm{J} \cdot \mathrm{T}^{-2}/\mathrm{erg} \cdot \mathrm{G}^{-2}) \times 10$, respectively.

$\langle b^2 \rangle - \langle a^2 \rangle =$	$-\ 24.8$	$\pm\ 1.2$
$\langle c^2 \rangle - \langle b^2 \rangle =$	$-\ 25.3$	$\pm\ 1.6$
$\langle a^2 \rangle - \langle c^2 \rangle =$	50.1	$\pm\ 2.2$
$\langle a^2 \rangle =$	55.9	$\pm\ 2.3$
$\langle b^2 \rangle =$	31.1	$\pm\ 1.7$
$\langle c^2 \rangle =$	5.8	$\pm\ 0.6$
$\chi_{aa}^{\mathrm{p}} =$	98.8	$\pm\ 2.1$
$\chi_{bb}^{\mathrm{p}} =$	205.4	$\pm\ 4.2$
$\chi_{cc}^{\mathrm{p}} =$	311.3	$\pm\ 4.7$
$\chi_{aa}^{\mathrm{d}} =$	$-\ 156.6$	$\pm\ 7.6$
$\chi_{bb}^{\mathrm{d}} =$	$-\ 261.7$	$\pm\ 10.0$
$\chi_{cc}^{\mathrm{d}} =$	$-\ 369.1$	$\pm\ 21.1$

The recalculated Zeeman parameters, after the above correction, are presented in Table 1.

In Table 3 of [2], due to a printing error, the sign of the molecular g-factor g_{aa} is reversed. It should read: $g_{aa} = -0.056 \pm 0.011$.

The new values of the in plane second moments $\langle a^2 \rangle$ and $\langle b^2 \rangle$ are comparable with those calculated by the additive formulae [1]. The still remaining discrepancy can be explained, from the experimentalists' side, as the molecular g-factors and the magnetic susceptibility anisotropies being particularly small for FClCO. In the range of the available magnetic fields they remain rather undetermined and therefore they introduce in the derived quantities considerable uncertainty, which may go beyond the estimated errors.

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[1] Z. B. Maksić and N. Mikac, Molec. Phys. **40**, 455 (1980).

[2] F. Scappini and A. Guarnieri, Z. Naturforsch. **31a**, 369 (1976).

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