Erratum: Influence of molecular orientation on the multiple differential cross sections for the $(e,2e)$ process on a water molecule [Phys. Rev. A **63, 052720 (2001)]**

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In the above paper, eightfold and fivefold differential cross sections (8DCS and 5DCS, respectively) have been calculated for the $(e,2e)$ process on a water molecule. This latter is described by means of five molecular orbitals expressed as an expansion of monocentric Slater-like functions centered on the oxygen atom [1]. However, Pr. Dal Cappello has recently pointed out that these molecular wave functions were not developed on a basis of complex spherical harmonics $Y_{lm}(r)$ but on a basis of real spherical harmonics $H_{lm}(r)$, which can be expressed as

$$H_{lm}(\hat{r}) = \left(\frac{m}{2|m|} \right)^{1/2} \left\{ Y_{l-|m|}(\hat{r}) + (-1)^m \left(\frac{m}{|m|} \right) Y_{l+|m|}(\hat{r}) \right\} \text{ if } m \neq 0, \\ H_{l0}(\hat{r}) = Y_{l0}(\hat{r}) \text{ if } m = 0. \quad (1)$$

FIG. 3. 8DCS calculated for water-molecule ionization at 250 eV (with an ejected electron of $E_e=5$ eV), in considering the contribution of each molecular orbital [the figures labeled from (a) to (d) correspond to the first, the second, the third, and the fourth molecular orbital, respectively]. The collision is studied in the coplanar geometry, i.e., $\varphi_e=\varphi_s=0^\circ$, and with a scattered angle θ_s of 0° . The different molecular orientations studied, denoted “parallel,” “antiparallel,” and “perpendicular” correspond to $(\alpha;\beta;\gamma)=(0^\circ;0^\circ;0^\circ)$, $(\alpha;\beta;\gamma)=(0^\circ;180^\circ;0^\circ)$, and $(\alpha;\beta;\gamma)=(0^\circ;90^\circ;90^\circ)$, respectively. They are represented by a solid line, a dashed line, and a dotted line, respectively.

FIG. 4. Same as Fig. 3 with $\theta_s = 15^\circ$.

Each molecular state labeled i is then described by the following wave function $\Psi_i(r)$ which replaces the expression given in Eqs. (3) and (4):

$$\Psi_i(\vec{r}) = \sum_{k=1}^{N_i} a_{ik} R_{n_{ik}}^{\xi_{ik}}(r) H_{l_{ik} m_{ik}}(r), \quad (2)$$

where N_i is the number of elements used to describe the i th molecular state ($N_i=7, 14, 7, 14$, and 14 for the orbital $1B_1, 3A_1, 1B_2, 2A_1$, and $1A_1$, respectively), and not the number of atomic states as it was initially noted.

In these conditions, Eq. (11) becomes

$$\begin{aligned} \left[\frac{d^8 \sigma}{d\alpha d\beta d\gamma d\Omega_s d\Omega_e dE_e} \right]_i &= \frac{32k_s}{k_i \cdot k_e \cdot q^4} \sum_{j,k=1}^{N_i} \sum_{\mu_j=-l_{ij}}^{l_{ij}} \sum_{\mu_k=-l_{ik}}^{l_{ik}} a_{ij} a_{ik} \\ &\times \left\{ \frac{D_{\mu_j - |m_{ij}|}^{(l_{ij})}(\alpha; \beta; \gamma) + (-1)^{m_{ij}} \left(\frac{m_{ij}}{|m_{ij}|} \right) D_{\mu_j |m_{ij}|}^{(l_{ij})}(\alpha; \beta; \gamma)}{\sqrt{2}} \right\} (1 - \delta_{m_{ij},0}) + D_{\mu_j 0}^{(l_{ij})}(\alpha; \beta; \gamma) \delta_{m_{ij},0} \Bigg\} \\ &\times \left\{ \frac{D_{\mu_k - |m_{ik}|}^{(l_{ik})}(\alpha; \beta; \gamma) + (-1)^{m_{ik}} \left(\frac{m_{ik}}{|m_{ik}|} \right) D_{\mu_k |m_{ik}|}^{(l_{ik})}(\alpha; \beta; \gamma)}{\sqrt{2}} \right\} (1 - \delta_{m_{ik},0}) + D_{\mu_k 0}^{(l_{ik})}(\alpha; \beta; \gamma) \delta_{m_{ik},0} \Bigg\}^* \\ &\times S_{n_{ij}, l_{ij}, m_{ij}}^{\mu_j} S_{n_{ik}, l_{ik}, m_{ik}}^{\mu_k}, \end{aligned} \quad (3)$$

where the S matrix is given by

FIG. 6. 5DCS calculated for different scattered angle values $\theta_s=0^\circ$ (a) and $\theta_s=15^\circ$ (b), respectively. The different subshell contributions are represented: the first MO (dot-dot-and-dashed line), the second MO (dot-and-dashed line), the third MO (dashed line), and the fourth MO (dotted line). The solid line corresponds to the “total” 5DCS.

$$S_{n_{ij}, l_{ij}, m_{ij}}^{\mu_j} = \sum_{l_e=0}^{\infty} \sum_{m_e=-l_e}^{l_e} \sum_{l=0}^{\infty} i^{(l-l_e)} e^{i\sigma_{l_e}} Y_{l_e m_e}(\hat{k}_e) (-1)^{\mu_j} Y_{l \mu_j - m_e}(\hat{q}) A_{l_{ij} m_{ij}}^{\mu_j} R_{l_e}^{n_{ij}, l_{ij}}. \quad (4)$$

The A matrix and the R matrix remain unchanged and are given by Eqs. (13) and (14), respectively. Finally, the 5DCS given in Eq. (17) and consequently in Eq. (19) become

$$\left[\frac{d^5\sigma}{d\Omega_s d\Omega_e dE_e} \right]_i = \frac{32k_s}{k_i \cdot k_e \cdot q^4} \sum_{j,k=1}^{N_i} \sum_{\mu_j=-l_{ij}}^{l_{ij}} \sum_{\mu_k=-l_{ik}}^{l_{ik}} \frac{a_{ij} a_{ik}}{l_{ij}} S_{n_{ij}, l_{ij}, m_{ij}}^{\mu_j} S_{n_{ik}, l_{ik}, m_{ik}}^{\mu_k*} \delta_{\mu_j, \mu_k} \delta_{l_{ij}, l_{ik}}. \quad (5)$$

By taking into account these modifications, we have reevaluated the 8DCS at $\theta_s=0^\circ$ and $\theta_s=15^\circ$ (Figs. 3 and 4, respectively). The observations made in the above paper remain valid. In particular, the shapes of the 8DCS do not really change and we still observe a quasi-atomic behavior for the different molecular states.

More precisely, the magnitudes of the 8DCS for the $1B_1$ and the $1B_2$ orbitals (which are “ $2p_{\pm 1}$ -like” orbitals) have sensitively changed but the minima are still observed at $\theta_e=0^\circ$, 180° , and 360° for the “parallel” and “antiparallel” configurations at $\theta_s=0^\circ$. However, for the “perpendicular” configuration, the minima which were previously located at $\theta_e=60^\circ$ and 240° are slightly shifted and are at present located at $\theta_e=90^\circ$ and 270° , which is more coherent considering the rotation of the target molecule. Let us note also that the contributions of the $1B_1$ orbital in the perpendicular configuration and that of the $1B_2$ orbital in the “parallel” and the “antiparallel” configurations (already very weak in the original paper) become now negligible.

Concerning the $3A_1$, which is predominantly governed by a $2p_0$ atomic orbital, the 8DCS remain unchanged, except for the “perpendicular” configuration, where minima are observed at $\theta_e=0^\circ$, 180° , and 360° instead of 150° and 320° in the previous work. Furthermore, let us note that these new minima correspond as expected to the maxima observed for the “parallel” and the “antiparallel” configurations.

For the $2A_1$ orbital, which is predominantly governed by a $2s$ atomic orbital (i.e., with a quantum number $m=0$), the 8DCS have not been affected by the substitution of the complex spherical harmonics $Y_{lm}(r)$ by the real spherical harmonics $H_{lm}(r)$ since according to Eq. (1), we have $H_{l0}(\hat{r})=Y_{l0}(\hat{r})$. Thus, the new wave function $\Psi_i(r)$ is, for this molecular orbital, quasi-identical to that previously published.

Similar observations can be made for the Fig. 4 where 8DCS at $\theta_s=15^\circ$ are reported.

Concerning Fig. 6, where 5DCS are reported, minor changes are observed.

For illustration, we report in the following the new two-dimensional Figs. 3, 4, and 6.

[1] R. Moccia, J. Chem. Phys. **40**, 2186 (1964).