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Errata

Use of Perturbation Methods for the Study of Configuration Interaction Effects

III. The Second Order Corrections to Transition Energies

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The expressions of the matrix elements between the monoexcited state $\frac{1}{\sqrt{2}}(p\bar{q}^* \pm q^*\bar{p})$ and the diexcited configurations $\begin{matrix} p & j^* \\ i & l^* \end{matrix}$ and $\begin{matrix} i & q^* \\ k & j^* \end{matrix}$ are wrong (p. 413 f.) and are equal to $[(q^*i|j^*l^*) - (q^*i|l^*j^*)]$, $[(i\ k|p\ j^*) - (i\ k|j^*p)]$.

One must change p into q^* and q^* into p in the numerators of Eq. (23) (p. 410). In the final expression of ΔE (p. 416 f.) one must change the first and second sum into

$$2\sum_{i<k}{}'\sum_{j^*}^{a}{}'\sum_{}^{b}{}'\left\{[(ik|q^*j^*)^2 + (ik|j^*q^*)^2 - (ik|q^*j^*)(ik|j^*q^*)]\frac{1}{\varepsilon_{j^*}+\varepsilon_{q^*}-\varepsilon_i-\varepsilon_k}\right.$$
$$\left. - [(ik|pj^*)^2 + (ik|j^*p)^2 - (ik|pj^*)(ik|j^*p)]\frac{1}{\varepsilon_{j^*}+\varepsilon_p-\varepsilon_i-\varepsilon_k}\right\}$$
$$+2\sum_{i}{}'\sum_{j^*<}^{a}{}'\sum_{l^*}^{b}{}'\left\{[(ip|j^*l^*)^2 + (ip|l^*j^*)^2 - (ip|j^*l^*)(ip|l^*j^*)]\frac{1}{\varepsilon_{j^*}+\varepsilon_{q^*}-\varepsilon_i-\varepsilon_p}\right.$$
$$\left. - [(iq^*|j^*l^*) + (iq^*|l^*j^*)^2 - (iq^*|j^*l^*)(iq^*|l^*j^*)]\frac{1}{\varepsilon_{j^*}+\varepsilon_{l^*}-\varepsilon_i-\varepsilon_{q^*}}\right\}$$

and the first two lines of the fifth sum into

$$\sum_{i}^{a}{}'\sum_{j^*}^{b}{}'\frac{(ii|q^*j^*)^2}{\varepsilon_{j^*}+\varepsilon_{q^*}-2\varepsilon_i} - \frac{(ii|pj^*)^2}{\varepsilon_{j^*}+\varepsilon_p-2\varepsilon_i} + \frac{(ip|j^*j^*)^2}{2\varepsilon_{j^*}-\varepsilon_i-\varepsilon_p} - \frac{(ip^*|j^*j^*)^2}{2\varepsilon_{j^*}-\varepsilon_i-\varepsilon_{q^*}}.$$

This change does not affect the main result and the selection rules of finally excited states are unchanged. The corollary remains valid.

Self Consistent Field Molecular Orbital Treatment Including Excited States of Cyclopropane, Ethylene Oxide and Ethyleneimine

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Reference [5] should read: Clark, P. A., and J. L. Ragle: J. chem. Physics **46**, 4325 (1967).