The corresponding contributions of the screened VP diagrams, depicted in Fig. 2(d)-(f), are

$$\Delta E_{\text{scrVP}}^{(b)a} = \Delta E_{\text{scrVP}}^{(0)} + \Delta E_{\text{scrVP}}^{(1, \text{irr})} + \Delta E_{\text{scrVP}}^{(1, \text{red})} + \Delta E_{\text{scrVP}}^{(1, b)},$$
(22)

$$\Delta E_{\text{scrVP}}^{(0)} = \langle a|U_{\text{VP}}|a\rangle - \langle a_{\text{C}}|U_{\text{VP}}|a_{\text{C}}\rangle, \qquad (23)$$

$$\Delta E_{\text{scrVP}}^{(1,\text{irr})} = 2 \sum_{b} \sum_{P} (-1)^{P} \left[\sum_{n}^{\varepsilon_{n} \neq \varepsilon_{a}} \frac{\langle PaPb | I(\Delta) | nb \rangle \langle n | U_{\text{VP}} | a \rangle}{\varepsilon_{a} - \varepsilon_{n}} + \sum_{n}^{\varepsilon_{n} \neq \varepsilon_{b}} \frac{\langle PaPb | I(\Delta) | an \rangle \langle n | U_{\text{VP}} | b \rangle}{\varepsilon_{b} - \varepsilon_{n}} \right] - 2 \sum_{n}^{\varepsilon_{n} \neq \varepsilon_{a}} \frac{\langle a | V_{\text{scr}} | n \rangle \langle n | U_{\text{VP}} | a \rangle}{\varepsilon_{a} - \varepsilon_{n}}, \quad (24)$$

$$\Delta E_{\text{scrVP}}^{(1, \text{ red})} = -\sum_{b} \sum_{P} (-1)^{P} \langle PaPb|I'(\Delta)|ab\rangle \left(\langle a|U_{\text{VP}}|a\rangle - \langle b|U_{\text{VP}}|b\rangle \right), \tag{25}$$

$$\Delta E_{\text{scrVP}}^{(1,b)} = \sum_{b} \sum_{P} (-1)^{P} \langle PaPb | I_{\text{VP}}(\Delta) | ab \rangle - \langle a | U_{\text{VP}}^{\text{scr}} | a \rangle, \qquad (26)$$

where $U_{\rm VP}$ denotes the VP potential, and $I_{\rm VP}(\Delta)$ is the interelectronic-interaction operator modified by the electron-loop. For the renormalization of the expressions (23)-(26) we refer to the works [5, 65]. Accordingly, these contributions are divided into the Uehling and Wichmann-Kroll parts. The renormalized Uehling parts of the VP operators $U_{\rm VP}$ and $I_{\rm VP}(\Delta)$ are given by the expressions (see, e.g., Ref. [5])

$$U_{\text{VP}}(r) = -\frac{2\alpha^2 Z}{3r} \int_1^\infty dt \, \frac{\sqrt{t^2 - 1}}{t^3} \left(1 + \frac{1}{2t^2} \right) \int_0^\infty dr' \, r' \rho_{\text{eff}}(r') \\ \times \left[\exp\left(-2|r - r'|t \right) - \exp\left(-2|r + r'|t \right) \right] , \tag{27}$$

$$I_{\rm VP}(\Delta, r_{12}) = \alpha \frac{\alpha_{1\mu} \alpha_2^{\mu}}{r_{12}} \frac{2\alpha}{3\pi} \int_1^{\infty} dt \, \frac{\sqrt{t^2 - 1}}{t^2} \left(1 + \frac{1}{2t^2} \right) \exp\left(-\sqrt{4t^2 - \Delta^2} \, r_{12}\right), \tag{28}$$

where the density $\rho_{\rm eff}$ is related to the nuclear binding and local screening potentials via the Poisson equation $\Delta V_{\rm nuc}(r) + \Delta V_{\rm scr}(r) = 4\pi\alpha Z\rho_{\rm eff}(r)$. $U_{\rm VP}^{\rm scr}$ differs from $U_{\rm VP}$ only by replacing $\rho_{\rm eff}$ with $\rho_{\rm scr}$, where the density $\rho_{\rm scr}$ is related to the screening potential $V_{\rm scr}$. The Wichmann-Kroll parts of the expressions (23)-(25) are evaluated employing the approximate formula for the Wichmann-Kroll potential [66]. The Wichmann-Kroll contribution to Eq. (26) is relatively small [5] and is neglected in the present consideration.

The numerical evaluation is based on the wave functions constructed from B-splines employing the dual-kinetic-balance finite basis set method [67]. The sphere model for the