One-electron operator coupling between two Slater determinants, $\left|\psi_a\right\rangle$ and $\left|\psi_b\right\rangle$:

$$\left\langle\psi_a\left|\hat{h}\right|\psi_b\right\rangle=\left(D_{aa}D_{bb}\right)^{-1}D_{ab}\sum_{i=1}^{N}\sum_{j=1}^{N}\left\langle\varphi_{ai}\left|\hat{h}\right|\varphi_{bj}\right\rangle(S_{ab}^{-1})_{ji},$$

where $\left\langle\varphi_{ai}\left|\hat{h}\right|\varphi_{bj}\right\rangle$ is the coupling between constituent orbitals, and D_{ab} is the determinant of overlap matrix defined as

$$D_{ab}=\begin{vmatrix}\left\langle\varphi_{a1}|\varphi_{b1}\right\rangle & \left\langle\varphi_{a1}|\varphi_{b2}\right\rangle & \cdots & \left\langle\varphi_{a1}|\varphi_{bN}\right\rangle\\ \left\langle\varphi_{a2}|\varphi_{b1}\right\rangle & \cdots & \cdots & \cdots\\ \cdots & \cdots & \cdots & \cdots\\ \left\langle\varphi_{aN}|\varphi_{b1}\right\rangle & \cdots & \cdots & \left\langle\varphi_{aN}|\varphi_{bN}\right\rangle\end{vmatrix}$$

The last term on the right-hand side S_{ab}^{-1} is the inverse of the overlap matrix.

Under the assumption of orthonormal orbitals, apparently, $D_{aa}=D_{bb}=1$.

Then, finally the expression can be simplified to

$$\left\langle\psi_a\left|\hat{h}\right|\psi_b\right\rangle=D_{ab}\sum_{i=1}^{N}\sum_{j=1}^{N}\left\langle\varphi_{ai}\left|\hat{h}\right|\varphi_{bj}\right\rangle(S_{ab}^{-1})_{ji},$$

please note the **index swap** between $\left\langle\varphi_{ai}\left|\hat{h}\right|\varphi_{bj}\right\rangle$ and $(S_{ab}^{-1})_{ji}$.

Reference:

Methods of Molecular Quantum Mechanics. Second Edition. (R. McWeeny, ISBN 0-12-486551-8), Page 66.