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Equation (63) of Ref. 1 is incomplete for the diagonal “semi-internal” configurations \( \Phi_{uu}^{ti} \). For the semi-internal configurations the contravariant functions defined in Eq. (61) take the explicit form

\[
\Phi_{uu}^{ti} = \frac{1}{2} \left[ \bar{e}_{ai} \bar{e}_{ai} + \delta_{iu} \left( \bar{e}_{ai} - \bar{e}_{ai} \right) \right] |0\rangle,
\]

which leads to

\[
\mathcal{V}_{uu}^{ti} = \frac{1}{2} \mathcal{V}_{uu}^{ti} + \frac{1}{2} \delta_{iu} (\bar{\mathcal{V}}_{u} - \bar{\mathcal{V}}_{u}).
\]

The second term, which contributes only for \( t = u \), was overlooked when deriving Eq. (63). A similar term should be added to Eq. (58). This means that the Schrödinger equation was projected with some functions that were not spin eigenfunctions. This has no effect if the wave function \( \Psi \) is a spin eigenfunction, as is the case for configuration interaction with single and double excitations (CISD). However, since the partially spin adapted coupled-cluster wave function based on spin-restricted orbitals (RHF-RCCSD) is spin adapted only in the linear terms, a small error results.

The contravariant functions \( \Phi_{uu}^{ti} \) in Eq. (1) are not orthogonal to the covariant functions defined by the operators in Eq. (48) of Ref. 1. More suitable contravariant functions, which fulfill the orthogonality condition, are

\[
\Phi_{uu}^{au} = \left[ \bar{e}_{ai} \bar{e}_{ai} + \delta_{iu} \left( \bar{e}_{ai} - \bar{e}_{ai} \right) \right] |0\rangle,
\]

where \( m \) is the number of open-shell orbitals. Using these configurations one obtains

\[
\langle \Phi_{uu}^{au} | \hat{T} | 0 \rangle = T_{uu}^{ti}
\]

and

\[
\mathcal{V}_{uu}^{ti} = \left[ \bar{V}_{uu}^{ti} + \delta_{iu} \left( \bar{V}_{u} - \bar{V}_{u} \right) \right] |0\rangle.
\]

Employing Eq. (2) or (5) yields the same solution, but by using Eq. (5) convergence is improved for states with triplet or higher spin multiplicity. The effect of the additional terms is very small, typically of the order of 0.01–0.1 mhartree. In all cases we have tested so far, the energy difference between

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Method</th>
<th>( E(r_e) )</th>
<th>( r_e / \text{Å} )</th>
<th>( B_r / \text{cm}^{-1} )</th>
<th>( \omega_r / \text{cm}^{-1} )</th>
<th>( \omega_{r,x} / \text{cm}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN(( ^2\Sigma^+ ))</td>
<td>RHF-UCCSD</td>
<td>-92.564 364 4</td>
<td>1.1646</td>
<td>1.924</td>
<td>2146.6</td>
<td>12.3</td>
</tr>
<tr>
<td>RHF-RCCSD</td>
<td>-92.563 315 1</td>
<td>1.1641</td>
<td>1.925</td>
<td>2148.3</td>
<td>12.4</td>
<td></td>
</tr>
<tr>
<td>RHF-RCCSD (Ref. 1)</td>
<td>-92.563 160 5</td>
<td>1.1641</td>
<td>1.925</td>
<td>2148.2</td>
<td>12.5</td>
<td></td>
</tr>
<tr>
<td>NO(( ^2\Pi ))</td>
<td>RHF-UCCSD</td>
<td>-129.724 331 9</td>
<td>1.1439</td>
<td>1.726</td>
<td>1986.5</td>
<td>12.9</td>
</tr>
<tr>
<td>RHF-RCCSD</td>
<td>-129.723 793 6</td>
<td>1.1435</td>
<td>1.727</td>
<td>1991.0</td>
<td>12.8</td>
<td></td>
</tr>
<tr>
<td>RHF-RCCSD (Ref. 1)</td>
<td>-129.723 729 5</td>
<td>1.1435</td>
<td>1.727</td>
<td>1991.9</td>
<td>12.7</td>
<td></td>
</tr>
<tr>
<td>O₂(( ^3\Sigma_u^+ ))</td>
<td>RHF-UCCSD</td>
<td>-150.141 733 5</td>
<td>1.1970</td>
<td>1.471</td>
<td>1677.7</td>
<td>10.2</td>
</tr>
<tr>
<td>RHF-RCCSD</td>
<td>-150.140 732 7</td>
<td>1.1964</td>
<td>1.473</td>
<td>1680.8</td>
<td>10.2</td>
<td></td>
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<tr>
<td>RHF-RCCSD (Ref. 1)</td>
<td>-150.140 618 1</td>
<td>1.1965</td>
<td>1.473</td>
<td>1680.2</td>
<td>10.2</td>
<td></td>
</tr>
</tbody>
</table>

*Basics cc-pVQZ (Ref. 4), but with highest angular momentum functions omitted (5s4p3d2f/4s3p2d); small deviations from RHF-UCCSD values in Table I of Ref. 1 can be attributed to the stricter convergence thresholds used here.
RHF-UCCSD (i.e., spin-restricted orbitals with unrestricted coupled-cluster amplitudes) and RHF-RCCSD is reduced.

The resulting partially spin adapted RCCSD method still differs from the ones described in Refs. 2 and 3 by the inclusion of the ‘‘disconnected’’ terms

\[ \Delta \tilde{V}_{pq} = \tilde{v}_p \tilde{q} \pi + \tilde{p}_p \tilde{q} \pi - \tilde{v}_q \tilde{p} \pi - \tilde{p}_q \tilde{v} \pi, \]

\[ \Delta \tilde{V}_{\bar{p}q} = \bar{v}_p \bar{q} \bar{\pi} + \bar{p}_p \bar{q} \bar{\pi} - \bar{v}_q \bar{p} \bar{\pi} - \bar{p}_q \bar{v} \bar{\pi}, \]

\[ \Delta V_{pq} = \tilde{v}_p \tilde{q} \pi + \tilde{p}_p \tilde{q} \pi - \tilde{q}_q \tilde{p} \pi - \tilde{q}_p \tilde{q} \pi, \]

in the residuals \( \tilde{V}_{pq}, \bar{V}_{pq}, \) and \( V_{pq} \), respectively. These terms vanish in the case of RHF-UCCSD, but give small contributions for RCCSD, since in this case the individual \( \tilde{v}_p \) and \( \bar{v}_p \) do not become zero for the converged solution. The appearance of these terms is not erroneous but is a consequence of the fact that we have not multiplied the Schrödinger equation from the left by \( \exp(-\hat{T}) \) before projection [cf. Eqs. (4)–(6) of Ref. 1]. For consistency with other programs we now recommend the removal of these terms as well, which typically cause energy changes of only a few microhartree.

Table I shows some results which can be compared with Table I of Ref. 1. The largest energy change is found for CN (0.15 mhartree). The change in the spectroscopic constants, however, is very small, and is almost within the error bounds of the polynomial fit of the potential energy curve. Similar results are obtained for the other molecules shown in Table I of Ref. 1. The corrected RHF-RCCSD method is identical to the partially spin adapted CCSD methods of Refs. 2 and 3.

We are indebted to Professor P. Botschwina for detecting the difference between results obtained with our previous program and those of Refs. 2 and 3, to Professor J. Gauss for pointing out to us the error in Eq. (63) of Ref. 1, and to Professor P. Szalay, Professor M. Urban, and Professor J. Gauss for providing test results for comparison.