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Supplementary Material. Symmetric Dissociation of the Water Molecule with Truncation Energy Error. A Benchmark Study

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I. EXPLICIT FORMULAE FOR THE $\mathrm{B_K}$ COEFFICIENTS

We give below the 64 formulae for the coefficients $\mathrm{B_K} = B_{i\dots}^{a\dots}$ of four-excited consolidated configurations $\mathrm{G_K}$ defined in Eq.(12) as the sum over all degenerate elements g of the configuration-state-functions F_{gK} of Eq.(11) used in the CI expansion Eq.(10). Their justification is provided in Sec.2.5.

$Case\ \ 1 : i < j < k < l \qquad a < b < c < d$

$$\begin{aligned} B_{ijkl}^{abcd} = {} & B_{ij}^{ab}B_{kl}^{cd} + B_{kl}^{ab}B_{ij}^{cd} - B_{ij}^{ac}B_{kl}^{bd} - B_{kl}^{ac}B_{ij}^{bd} + B_{ij}^{ad}B_{kl}^{bc} + B_{kl}^{ad}B_{ij}^{bc} - \\ & B_{ik}^{ab}B_{jl}^{cd} - B_{jl}^{ab}B_{ik}^{cd} + B_{ik}^{ac}B_{jl}^{bd} + B_{jl}^{ac}B_{ik}^{bd} - B_{ik}^{ad}B_{jl}^{bc} - B_{jl}^{ad}B_{ik}^{bc} + \\ & B_{il}^{ab}B_{jk}^{cd} + B_{jk}^{ab}B_{il}^{cd} - B_{il}^{ac}B_{jk}^{bd} - B_{jk}^{ac}B_{il}^{bd} + B_{il}^{ad}B_{jk}^{bc} + B_{jk}^{ad}B_{il}^{bc} \end{aligned} \tag{1}$$

$Case\ \ 2 : i < j < k < l \qquad a = b < c < d$

$$\begin{aligned} B_{ijkl}^{aacd} = {} & B_{ij}^{aa}B_{kl}^{cd} + B_{kl}^{aa}B_{ij}^{cd} - B_{ij}^{ac}B_{kl}^{ad} - B_{kl}^{ac}B_{ij}^{ad} - B_{ik}^{aa}B_{jl}^{cd} - B_{jl}^{aa}B_{ik}^{cd} + \\ & B_{ik}^{ac}B_{jl}^{ad} + B_{jl}^{ac}B_{ik}^{ad} + B_{il}^{aa}B_{jk}^{cd} + B_{jk}^{aa}B_{il}^{cd} - B_{il}^{ac}B_{jk}^{ad} - B_{jk}^{ac}B_{il}^{ad} \end{aligned} \tag{2}$$

$Case\ \ 3 : i < j < k < l \qquad a < b = c < d$

$$\begin{aligned} B_{ijkl}^{abbd} = {} & B_{ij}^{ab}B_{kl}^{bd} + B_{kl}^{ab}B_{ij}^{bd} + B_{ij}^{ad}B_{kl}^{bb} + B_{kl}^{ad}B_{ij}^{bb} - B_{ik}^{ab}B_{jl}^{bd} - B_{jl}^{ab}B_{ik}^{bd} - \\ & B_{ik}^{ad}B_{jl}^{bb} - B_{jl}^{ad}B_{ik}^{bb} + B_{il}^{ab}B_{jk}^{bd} + B_{jk}^{ab}B_{il}^{bd} + B_{il}^{ad}B_{jk}^{bb} + B_{jk}^{ad}B_{il}^{bb} \end{aligned} \tag{3}$$

$Case\ \ 4 : i < j < k < l \qquad a < b < c = d$

$$\begin{aligned} B_{ijkl}^{abcc} = {} & B_{ij}^{ab}B_{kl}^{cc} + B_{kl}^{ab}B_{ij}^{cc} - B_{ij}^{ac}B_{kl}^{bc} - B_{kl}^{ac}B_{ij}^{bc} - B_{ik}^{ab}B_{jl}^{cc} - B_{jl}^{ab}B_{ik}^{cc} + \\ & B_{ik}^{ac}B_{jl}^{bc} + B_{jl}^{ac}B_{ik}^{bc} + B_{il}^{ab}B_{jk}^{cc} + B_{jk}^{ab}B_{il}^{cc} - B_{il}^{ac}B_{jk}^{bc} - B_{jk}^{ac}B_{il}^{bc} \end{aligned} \tag{4}$$

$Case\ \ 5 : i < j < k < l \qquad a = b < c = d$

$$\begin{aligned} B_{ijkl}^{aacc} = {} & B_{ij}^{aa}B_{kl}^{cc} + B_{kl}^{aa}B_{ij}^{cc} - B_{ij}^{ac}B_{kl}^{ac} - B_{ik}^{aa}B_{jl}^{cc} - B_{jl}^{aa}B_{ik}^{cc} + B_{ik}^{ac}B_{jl}^{ac} + \\ & B_{il}^{aa}B_{jk}^{cc} + B_{jk}^{aa}B_{il}^{cc} - B_{il}^{ac}B_{jk}^{ac} \end{aligned} \tag{5}$$

$Case\ \ 6 : i < j < k < l \qquad a = b = c < d$

$$B_{ijkl}^{aaad} = B_{ij}^{aa}B_{kl}^{ad} + B_{kl}^{aa}B_{ij}^{ad} - B_{ik}^{aa}B_{jl}^{ad} - B_{jl}^{aa}B_{ik}^{ad} + B_{il}^{aa}B_{jk}^{ad} + B_{jk}^{aa}B_{il}^{ad} \tag{6}$$

$Case\ \ 7 : i < j < k < l \qquad a < b = c = d$

$$B^{abbb}_{ijkl} = B^{ab}_{ij}B^{bb}_{kl} + B^{ab}_{kl}B^{bb}_{ij} - B^{ab}_{ik}B^{bb}_{jl} - B^{ab}_{jl}B^{bb}_{ik} + B^{ab}_{il}B^{bb}_{jk} + B^{ab}_{jk}B^{bb}_{il} \tag{7}$$

$Case\ \ 8 : i < j < k < l \qquad a = b = c = d$

$$B^{aaaa}_{ijkl} = B^{aa}_{ij}B^{aa}_{kl} - B^{aa}_{ik}B^{aa}_{jl} + B^{aa}_{il}B^{aa}_{jk} \tag{8}$$

$Case\ \ 9 : i = j < k < l \qquad a < b < c < d$

$$\begin{aligned} B^{abcd}_{iikl} = B^{ab}_{ii}B^{cd}_{kl} + B^{ab}_{kl}B^{cd}_{ii} - B^{ac}_{ii}B^{bd}_{kl} - B^{ac}_{kl}B^{bd}_{ii} + B^{ad}_{ii}B^{bc}_{kl} + B^{ad}_{kl}B^{bc}_{ii} - \\ B^{ab}_{ik}B^{cd}_{il} - B^{ab}_{il}B^{cd}_{ik} + B^{ac}_{ik}B^{bd}_{il} + B^{ac}_{il}B^{bd}_{ik} - B^{ad}_{ik}B^{bc}_{il} - B^{ad}_{il}B^{bc}_{ik} \end{aligned} \tag{9}$$

$Case\ \ 10 : i = j < k < l \qquad a = b < c < d$

$$\begin{aligned} B^{aacd}_{iikl} = B^{aa}_{ii}B^{cd}_{kl} + B^{aa}_{kl}B^{cd}_{ii} - B^{ac}_{ii}B^{ad}_{kl} - B^{ac}_{kl}B^{ad}_{ii} - B^{aa}_{ik}B^{cd}_{il} - B^{aa}_{il}B^{cd}_{ik} + \\ B^{ac}_{ik}B^{ad}_{il} + B^{ac}_{il}B^{ad}_{ik} \end{aligned} \tag{10}$$

$Case\ \ 11 : i = j < k < l \qquad a < b = c < d$

$$\begin{aligned} B^{abbd}_{iikl} = B^{ab}_{ii}B^{bd}_{kl} + B^{ab}_{kl}B^{bd}_{ii} + B^{ad}_{ii}B^{bb}_{kl} + B^{ad}_{kl}B^{bb}_{ii} - B^{ab}_{ik}B^{bd}_{il} - B^{ab}_{il}B^{bd}_{ik} - \\ B^{ad}_{ik}B^{bb}_{il} - B^{ad}_{il}B^{bb}_{ik} \end{aligned} \tag{11}$$

$Case\ \ 12 : i = j < k < l \qquad a < b < c = d$

$$\begin{aligned} B^{abcc}_{iikl} = B^{ab}_{ii}B^{cc}_{kl} + B^{ab}_{kl}B^{cc}_{ii} - B^{ac}_{ii}B^{bc}_{kl} - B^{ac}_{kl}B^{bc}_{ii} - B^{ab}_{ik}B^{cc}_{il} - B^{ab}_{il}B^{cc}_{ik} + \\ B^{ac}_{ik}B^{bc}_{il} + B^{ac}_{il}B^{bc}_{ik} \end{aligned} \tag{12}$$

$Case\ \ 13 : i = j < k < l \qquad a = b < c = d$

$$B^{aacc}_{iikl} = B^{aa}_{ii}B^{cc}_{kl} + B^{aa}_{kl}B^{cc}_{ii} - B^{ac}_{ii}B^{ac}_{kl} - B^{aa}_{ik}B^{cc}_{il} - B^{aa}_{il}B^{cc}_{ik} + B^{ac}_{ik}B^{ac}_{il} \tag{13}$$

$Case\ \ 14 : i = j < k < l \qquad a = b = c < d$

$$B^{aaad}_{iikl} = B^{aa}_{ii}B^{ad}_{kl} + B^{ad}_{ii}B^{aa}_{kl} - B^{aa}_{ik}B^{ad}_{il} - B^{ad}_{ik}B^{aa}_{il} \tag{14}$$

$Case\ \ 15 : i = j < k < l \qquad a < b = c = d$

$$B^{abbb}_{iikl} = B^{ab}_{ij} B^{cd}_{kl} + B^{cd}_{ij} B^{ab}_{kl} - B^{ab}_{ik} B^{cd}_{jl} - B^{cd}_{ik} B^{ab}_{jl} \tag{15}$$

$Case\ \ 16 : i = j < k < l \qquad a = b = c = d$

$$B^{aaaa}_{iikl} = B^{aa}_{ii} B^{aa}_{kl} - B^{aa}_{ik} B^{aa}_{il} \tag{16}$$

$Case\ \ 17 : i < j = k < l \qquad a < b < c < d$

$$\begin{aligned} B^{abcd}_{ijjl} = {} & B^{ab}_{jj} B^{cd}_{il} + B^{ab}_{il} B^{cd}_{jj} - B^{ac}_{jj} B^{bd}_{il} - B^{ac}_{il} B^{bd}_{jj} + B^{ad}_{jj} B^{bc}_{il} + B^{ad}_{il} B^{bc}_{jj} - \\ & B^{ab}_{ij} B^{cd}_{jl} - B^{ab}_{jl} B^{cd}_{ij} + B^{ac}_{ij} B^{bd}_{jl} + B^{ac}_{jl} B^{bd}_{ij} - B^{ad}_{ij} B^{bc}_{jl} - B^{ad}_{jl} B^{bc}_{ij} \end{aligned} \tag{17}$$

$Case\ \ 18 : i < j = k < l \qquad a = b < c < d$

$$\begin{aligned} B^{aacd}_{ijjl} = {} & B^{aa}_{jj} B^{cd}_{il} + B^{aa}_{il} B^{cd}_{jj} - B^{ac}_{jj} B^{ad}_{il} + B^{ac}_{il} B^{ad}_{jj} - B^{aa}_{ij} B^{cd}_{jl} - B^{aa}_{jl} B^{cd}_{ij} + \\ & B^{ac}_{ij} B^{ad}_{jl} - B^{ac}_{jl} B^{ad}_{ij} \end{aligned} \tag{18}$$

$Case\ \ 19 : i < j = k < l \qquad a < b = c < d$

$$\begin{aligned} B^{abbd}_{ijjl} = {} & B^{ab}_{jj} B^{bd}_{il} + B^{ab}_{il} B^{bd}_{jj} + B^{ad}_{jj} B^{bb}_{il} + B^{ad}_{il} B^{bb}_{jj} - B^{ab}_{ij} B^{bd}_{jl} - B^{ab}_{jl} B^{bd}_{ij} - \\ & B^{ad}_{ij} B^{bb}_{jl} - B^{ad}_{jl} B^{bb}_{ij} \end{aligned} \tag{19}$$

$Case\ \ 20 : i < j = k < l \qquad a < b < c = d$

$$\begin{aligned} B^{abcc}_{ijjl} = {} & B^{ab}_{jj} B^{cc}_{il} + B^{ab}_{il} B^{cc}_{jj} - B^{ac}_{jj} B^{bc}_{il} - B^{ac}_{il} B^{bc}_{jj} - B^{ab}_{ij} B^{cc}_{jl} - B^{ab}_{jl} B^{cc}_{ij} + \\ & B^{ac}_{ij} B^{bc}_{jl} + B^{ac}_{jl} B^{bc}_{ij} \end{aligned} \tag{20}$$

$Case\ \ 21 : i < j = k < l \qquad a = b < c = d$

$$B^{aacc}_{ijjl} = B^{aa}_{jj} B^{cc}_{il} + B^{aa}_{il} B^{cc}_{jj} - B^{ac}_{jj} B^{ac}_{il} - B^{aa}_{ij} B^{cc}_{jl} - B^{aa}_{jl} B^{cc}_{ij} + B^{ac}_{ij} B^{ac}_{jl} \tag{21}$$

$Case\ \ 22 : i < j = k < l \qquad a = b = c < d$

$$B_{ijjl}^{aaad} = B_{jj}^{aa} B_{il}^{ad} + B_{jj}^{ad} B_{il}^{aa} - B_{ij}^{aa} B_{jl}^{ad} - B_{ij}^{ad} B_{jl}^{aa} \tag{22}$$

$Case\ \ 23 : i < j = k < l \qquad a < b = c = d$

$$B_{ijjl}^{abbb} = B_{jj}^{ab} B_{il}^{bb} + B_{jj}^{bb} B_{il}^{ab} - B_{ij}^{ab} B_{jl}^{bb} - B_{ij}^{bb} B_{jl}^{ab} \tag{23}$$

$Case\ \ 24 : i < j = k < l \qquad a = b = c = d$

$$B_{ijjl}^{aaaa} = B_{jj}^{aa} B_{il}^{aa} - B_{ij}^{aa} B_{jl}^{aa} \tag{24}$$

$Case\ \ 25 : i < j < k = l \qquad a < b < c < d$

$$\begin{aligned} B_{ijkk}^{abcd} = B_{ij}^{ab} B_{kk}^{cd} + B_{kk}^{ab} B_{ij}^{cd} - B_{ij}^{ac} B_{kk}^{bd} - B_{kk}^{ac} B_{ij}^{bd} + B_{ij}^{ad} B_{kk}^{bc} + B_{kk}^{ad} B_{ij}^{bc} - \\ B_{ik}^{ab} B_{jk}^{cd} - B_{jk}^{ab} B_{ik}^{cd} + B_{ik}^{ac} B_{jk}^{bd} + B_{jk}^{ac} B_{ik}^{bd} - B_{ik}^{ad} B_{jk}^{bc} - B_{jk}^{ad} B_{ik}^{bc} \end{aligned} \tag{25}$$

$Case\ \ 26 : i < j < k = l \qquad a = b < c < d$

$$\begin{aligned} B_{ijkk}^{aacd} = B_{ij}^{aa} B_{kk}^{cd} + B_{kk}^{aa} B_{ij}^{cd} - B_{ij}^{ac} B_{kk}^{ad} - B_{kk}^{ac} B_{ij}^{ad} - B_{ik}^{aa} B_{jk}^{cd} - B_{jk}^{aa} B_{ik}^{cd} + \\ B_{ik}^{ac} B_{jk}^{ad} + B_{jk}^{ac} B_{ik}^{ad} \end{aligned} \tag{26}$$

$Case\ \ 27 : i < j < k = l \qquad a < b = c < d$

$$\begin{aligned} B_{ijkk}^{abbd} = B_{ij}^{ab} B_{kk}^{bd} + B_{kk}^{ab} B_{ij}^{bd} + B_{ij}^{ad} B_{kk}^{bb} + B_{kk}^{ad} B_{ij}^{bb} - B_{ik}^{ab} B_{jk}^{bd} - B_{jk}^{ab} B_{ik}^{bd} - \\ B_{ik}^{ad} B_{jk}^{bb} - B_{jk}^{ad} B_{ik}^{bb} \end{aligned} \tag{27}$$

$Case\ \ 28 : i < j < k = l \qquad a < b < c = d$

$$\begin{aligned} B_{ijkk}^{abcc} = B_{ij}^{ab} B_{kk}^{cc} + B_{kk}^{ab} B_{ij}^{cc} - B_{ij}^{ac} B_{kk}^{bc} - B_{kk}^{ac} B_{ij}^{bc} - B_{ik}^{ab} B_{jk}^{cc} - B_{jk}^{ab} B_{ik}^{cc} + \\ B_{ik}^{ac} B_{jk}^{bc} + B_{jk}^{ac} B_{ik}^{bc} \end{aligned} \tag{28}$$

$Case\ \ 29 : i < j < k = l \qquad a = b < c = d$

$$B^{aacc}_{ijkk} = B^{aa}_{ij} B^{cc}_{kk} + B^{aa}_{kk} B^{cc}_{ij} - B^{ac}_{ij} B^{ac}_{kk} - B^{aa}_{ik} B^{cc}_{jk} - B^{aa}_{jk} B^{cc}_{ik} + B^{ac}_{ik} B^{ac}_{jk} \tag{29}$$

$Case\ \ 30 : i < j < k = l \qquad a = b = c < d$

$$B^{aaad}_{ijkk} = B^{aa}_{ij} B^{ad}_{kk} + B^{ad}_{ij} B^{aa}_{kk} - B^{aa}_{ik} B^{ad}_{jk} - B^{ad}_{ik} B^{aa}_{jk} \tag{30}$$

$Case\ \ 31 : i < j < k = l \qquad a < b = c = d$

$$B^{abbb}_{ijkk} = B^{ab}_{ij} B^{bb}_{kk} + B^{bb}_{ij} B^{ab}_{kk} - B^{ab}_{ik} B^{bb}_{jk} - B^{bb}_{ik} B^{ab}_{jk} \tag{31}$$

$Case\ \ 32 : i < j < k = l \qquad a = b = c = d$

$$B^{aaaa}_{ijkk} = B^{aa}_{ij} B^{aa}_{kk} - B^{aa}_{ik} B^{aa}_{jk} \tag{32}$$

$Case\ \ 33 : i = j < k = l \qquad a < b < c < d$

$$\begin{aligned} B^{abcd}_{iikk} = B^{ab}_{ii} B^{cd}_{kk} + B^{ab}_{kk} B^{cd}_{ii} - B^{ac}_{ii} B^{bd}_{kk} - B^{ac}_{kk} B^{bd}_{ii} + B^{ad}_{ii} B^{bc}_{kk} + B^{ad}_{kk} B^{bc}_{ii} - \\ B^{ab}_{ik} B^{cd}_{ik} - B^{ac}_{ik} B^{bd}_{ik} + B^{ad}_{ik} B^{bc}_{ik} \end{aligned} \tag{33}$$

$Case\ \ 34 : i = j < k = l \qquad a = b < c < d$

$$B^{aacd}_{iikk} = B^{aa}_{ii} B^{cd}_{kk} + B^{aa}_{kk} B^{cd}_{ii} - B^{ac}_{ii} B^{ad}_{kk} - B^{ac}_{kk} B^{ad}_{ii} - B^{aa}_{ik} B^{cd}_{ik} + B^{ac}_{ik} B^{ad}_{ik} \tag{34}$$

$Case\ \ 35 : i = j < k = l \qquad a < b = c < d$

$$B^{abbd}_{iikk} = B^{ab}_{ii} B^{bd}_{kk} + B^{ab}_{kk} B^{bd}_{ii} + B^{ad}_{ii} B^{bb}_{kk} + B^{ad}_{kk} B^{bb}_{ii} - B^{ab}_{ik} B^{bd}_{ik} - B^{ad}_{ik} B^{bb}_{ik} \tag{35}$$

$Case\ \ 36 : i = j < k = l \qquad a < b < c = d$

$$B^{abcc}_{iikk} = B^{ab}_{ii} B^{cc}_{kk} + B^{ab}_{kk} B^{cc}_{ii} - B^{ac}_{ii} B^{bc}_{kk} - B^{ac}_{kk} B^{bc}_{ii} - B^{ab}_{ik} B^{cc}_{ik} + B^{ac}_{ik} B^{bc}_{ik} \tag{36}$$

$Case\ \ 37 : i = j < k = l \qquad a = b < c = d$

$$B^{aacc}_{iikk} = B^{aa}_{ii}B^{cc}_{kk} + B^{aa}_{kk}B^{cc}_{ii} - B^{ac}_{ii}B^{ac}_{kk} - B^{aa}_{ik}B^{cc}_{ik} + B^{ac}_{ik}B^{ac}_{ik} \tag{37}$$

$Case\ \ 38 : i = j < k = l \qquad a = b = c < d$

$$B^{aaad}_{iikk} = B^{aa}_{ii}B^{ad}_{kk} - B^{aa}_{kk}B^{ad}_{ii} + B^{aa}_{ik}B^{ad}_{ik} \tag{38}$$

$Case\ \ 39 : i = j < k = l \qquad a < b = c = d$

$$B^{abbb}_{iikk} = B^{ab}_{ii}B^{bb}_{kk} - B^{ab}_{kk}B^{bb}_{ii} + B^{ab}_{ik}B^{bb}_{ik} \tag{39}$$

$Case\ \ 40 : i = j < k = l \qquad a = b = c = d$

$$B^{aaaa}_{iikk} = B^{aa}_{ii}B^{aa}_{kk} - B^{aa}_{ik}B^{aa}_{ik} \tag{40}$$

$Case\ \ 41 : i = j = k < l \qquad a < b < c < d$

$$B^{abcd}_{iiil} = B^{ab}_{ii}B^{cd}_{il} + B^{ab}_{il}B^{cd}_{ii} - B^{ac}_{ii}B^{bd}_{il} - B^{ac}_{il}B^{bd}_{ii} + B^{ad}_{ii}B^{bc}_{il} + B^{ad}_{il}B^{bc}_{ii} \tag{41}$$

$Case\ \ 42 : i = j = k < l \qquad a = b < c < d$

$$B^{aacd}_{iiil} = B^{aa}_{ii}B^{cd}_{il} + B^{aa}_{il}B^{cd}_{ii} - B^{ac}_{ii}B^{ad}_{il} - B^{ac}_{il}B^{ad}_{ii} \tag{42}$$

$Case\ \ 43 : i = j = k < l \qquad a < b = c < d$

$$B^{abbd}_{iiil} = B^{ab}_{ii}B^{bd}_{il} + B^{ab}_{il}B^{bd}_{ii} - B^{ad}_{ii}B^{bb}_{il} - B^{ad}_{il}B^{bb}_{ii} \tag{43}$$

$Case\ \ 44 : i = j = k < l \qquad a < b < c = d$

$$B^{abcc}_{iiil} = B^{ab}_{ii}B^{cc}_{il} + B^{ab}_{il}B^{cc}_{ii} - B^{ac}_{ii}B^{bc}_{il} - B^{ac}_{il}B^{bc}_{ii} \tag{44}$$

$Case\ \ 45 : i = j = k < l \qquad a = b < c = d$

$$B^{aacc}_{iiil} = B^{aa}_{ii}B^{cc}_{il} + B^{aa}_{il}B^{cc}_{ii} - B^{ac}_{ii}B^{ac}_{il} \tag{45}$$

$Case\ \ 46 : i = j = k < l \qquad a = b = c < d$

$$B^{aaad}_{iiil} = B^{aa}_{ii}B^{ad}_{il} + B^{aa}_{il}B^{ad}_{ii} \tag{46}$$

$Case\ \ 47 : i = j = k < l \qquad a < b = c = d$

$$B^{abbb}_{iiil} = B^{ab}_{ii}B^{bb}_{il} + B^{ab}_{il}B^{bb}_{ii} \tag{47}$$

$Case\ \ 48 : i = j = k < l \qquad a = b = c = d$

$$B^{aaaa}_{iiil} = B^{aa}_{ii}B^{aa,il} \tag{48}$$

$Case\ \ 49 : i < j = k = l \qquad a < b < c < d$

$$B^{abcd}_{ijjj} = B^{ab}_{ij}B^{cd}_{jj} + B^{ab}_{jj}B^{cd}_{ij} - B^{ac}_{ij}B^{bd}_{jj} - B^{ac}_{jj}B^{bd}_{ij} + B^{ad}_{ij}B^{bc}_{jj} + B^{ad}_{jj}B^{bc}_{ij} \tag{49}$$

$Case\ \ 50 : i < j = k = l \qquad a = b < c < d$

$$B^{aacd}_{ijjj} = B^{aa}_{ij}B^{cd}_{jj} + B^{aa}_{jj}B^{cd}_{ij} - B^{ac}_{ij}B^{ad}_{jj} - B^{ac}_{jj}B^{ad}_{ij} \tag{50}$$

$Case\ \ 51 : i < j = k = l \qquad a < b = c < d$

$$B^{abbd}_{ijjj} = B^{ab}_{ij}B^{bd}_{jj} + B^{ab}_{jj}B^{bd}_{ij} + B^{ad}_{ij}B^{bb}_{jj} + B^{ad}_{jj}B^{bb}_{ij} \tag{51}$$

$Case\ \ 52 : i < j = k = l \qquad a < b < c = d$

$$B^{abcc}_{ijjj} = B^{ab}_{ij}B^{cc}_{jj} + B^{ab}_{jj}B^{cc}_{ij} - B^{ac}_{ij}B^{bc}_{jj} - B^{ac}_{jj}B^{bc}_{ij} \tag{52}$$

$Case\ \ 53 : i < j = k = l \qquad a = b < c = d$

$$B^{aacc}_{ijjj} = B^{aa}_{ij}B^{cc}_{jj} + B^{aa}_{jj}B^{cc}_{ij} - B^{ac}_{ij}B^{ac}_{jj} \tag{53}$$

$Case\ \ 54 : i < j = k = l \qquad a = b = c < d$

$$B^{aaad}_{ijjj} = B^{aa}_{ij}B^{ad}_{jj} + B^{aa}_{jj}B^{ad}_{ij} \tag{54}$$

$Case\ \ 55 : i < j = k = l \qquad a < b = c = d$

$$B^{abbb}_{ijjj} = B^{ab}_{ij}B^{bb}_{jj} + B^{ab}_{jj}B^{bb}_{ij} \tag{55}$$

$Case\ \ 56 : i < j = k = l \quad\quad a = b = c = d$

$$B^{aaaa}_{ijjj} = B^{aa}_{ij} B^{aa}_{jj} \tag{56}$$

$Case\ \ 57 : i = j = k = l \quad\quad a < b < c < d$

$$B^{abcd}_{iiii} = B^{ab}_{ii} B^{cd}_{ii} - B^{ac}_{ii} B^{bd}_{ii} + B^{ad}_{ii} B^{bc}_{ii} \tag{57}$$

$Case\ \ 58 : i = j = k = l \quad\quad a = b < c < d$

$$B^{aacd}_{iiii} = B^{aa}_{ii} B^{cd}_{ii} - B^{ac}_{ii} B^{ad}_{ii} \tag{58}$$

$Case\ \ 59 : i = j = k = l \quad\quad a < b = c < d$

$$B^{abbd}_{iiii} = B^{ab}_{ii} B^{bd}_{ii} + B^{ad}_{ii} B^{bb}_{ii} \tag{59}$$

$Case\ \ 60 : i = j = k = l \quad\quad a < b < c = d$

$$B^{abcc}_{iiii} = B^{ab}_{ii} B^{cc}_{ii} - B^{ac}_{ii} B^{bc}_{ii} \tag{60}$$

$Case\ \ 61 : i = j = k = l \quad\quad a = b < c = d$

$$B^{aacc}_{iiii} = B^{aa}_{ii} B^{cc}_{ii} - B^{ac}_{ii} B^{ac}_{ii} \tag{61}$$

$Case\ \ 62 : i = j = k = l \quad\quad a = b = c < d$

$$B^{aaad}_{iiii} = B^{aa}_{ii} B^{ad}_{ii} \tag{62}$$

$Case\ \ 63 : i = j = k = l \quad\quad a < b = c = d$

$$B^{abbb}_{iiii} = B^{ab}_{ii} B^{bb}_{ii} \tag{63}$$

$Case\ \ 64 : i = j = k = l \quad\quad a = b = c = d$

$$B^{aaaa}_{iiii} = B^{aa}_{ii} B^{aa}_{ii} \tag{64}$$

II. DETAILS OF A SCI-TEE CALCULATION

For a given orbital basis and geometry, program NWChem [1] is used to calculate an SCF wave function and a corresponding list of one- and two-electron integrals. A copy of these integrals will be saved from which new integral lists will be produced by program ATMOL where the original orbitals are transformed into some kind of natural orbitals.

The next step is to shorten a huge model space $\mathcal{M}$ into a pruned space $\mathcal{P}$ where most subclasses and configurations are discarded with TEEs giving a fair idea about needed resources for variational calculations of given accuracy. This step was not deemed necessary for the relatively small triple-ζ bases used. Therefore, the TEE $\Delta E^{\mathrm{FCI}}_{\mathcal{M}\to\mathcal{P}}$=0.

Since the pruning of $\mathcal{M}$ into $\mathcal{P}$ was omitted, the next step becomes concurrent with the development of suitable natural orbitals NO-nx, which otherwise would have been evaluated earlier. Each time a new NO-nx basis is obtained, the B_{K} CI coefficients CIC-nx of Eq.(12) to evaluate TEEs by Eqs.(15,17,19,20) are also updated.

Program AUTOCL is used to produce a list of symmetry eigenfunctions up to CI-2x which is used by ATMOL to get natural orbitals NO-2x. Using NO-2x, another CI-2x gives CI coefficients CIC-2x, which together with the integrals from NWChem can be used by AUTOCL to prune a CI-3x or CI-4x list using various selection thresholds aiming to produce a compact SCI-TEE-nx with a suitable TEE from which to get NO-nx. We settled on a NO-3x basis obtained from a CI-3x. Larger orbital sets would require the use of SCI-TEE-nx instead of CI-nx, and even the pruning of $\mathcal{M}$ into $\mathcal{P}$.

With the NO-3x, we now produce a compact space $\mathcal{S}$ selected according to tight and numerous thresholds given explicitly in the next section. The aim is to produce moderate numbers of nonzero matrix elements and sufficiently small TEEs $\Delta E^{\mathrm{FCI}}_{\mathcal{P}\to\mathcal{S}}$. This is achieved through inquiring for TEEs obtained with various sets of selection thresholds in Sec.3 1 combined with the cost-effectiveness thresholds of Eqs.(22-23). For the present calculations, each inquiring of TEEs takes less than one minute on a well equipped laptop, since no variational calculations are involved. The selection thresholds used at equilibrium geometry proved to be suitable for all other internuclear distances, yielding TEEs below 2 μHartree, which increase to 10 μHartree after including ΔECIBP.

This step requires setting two variables: the maximum CI size in CIBP on RAM, S^{CIBP}, and the RAM size allocated to nonzero Hamiltonian matrix elements and corresponding indices, S^{HMT}. Their values will decide if $\mathcal{S}_{01}$ is computed in RAM, and whether the successive CIBP matrices and indices will fit in RAM. Typical values are S^{CIBP}=300000 and S^{HMT}=20GB on a 32 GB laptop, or S^{CIBP}=2000000 and S^{HMT}=200GB on a 256 GB computer node.

The rest consists of a large-scale variational calculation usually combined with CIBP using program ATMOL without further human intervention.

III. SELECTION THRESHOLDS ON THE PRUNED CONFIGURATION LIST

We have used a single and compact set of selection threshold values for all calculations. In general, we used $\mathcal{T}_{\rm c}^{\rm ps}(q)$=$\mathcal{T}_{\rm d}^{\rm ps}(q)$ for all q. For the $\mathcal{S}_0$ space we used (in a.u.) $\mathcal{T}^{\rm br}(q)$=$\mathcal{T}_{\rm d}^{\rm ps}(q)$=$10^{-8}$ for q=1,2 and 10^{-6} for q=3-6. The $\mathcal{S}_1$ space is selected by $\mathcal{T}^{\rm br}(q)$=10^{-12}, $\mathcal{T}_{\rm d}^{\rm ps}(q)$=$10^{-10}$ for q=1,2, and 10^{-10},10^{-8} for q=3-6, respectively. The $\mathcal{S}_r$ space is selected by $\mathcal{T}^{\rm br}(q)$=10^{-16}, $\mathcal{T}_{\rm d}^{\rm ps}(q)$=$10^{-12}$ for q=1,2, and 10^{-14},10^{-10} for q=3-6, respectively. The above drastically reduces the number of different threshold values from those in our previous work. Successive applications of the SCI-TEE process are helped by a shell script linking a sequence of runs, aiming at developing a simple protocol to run SCI-TEE in a black box manner.

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