

BSSE for Trimers: Expression, Term Analysis, and Study Plan

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Abstract

A concise, modular document outlining the BSSE formulation for a trimer, a short analysis of its terms, and the computational plan for our study.

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1. BSSE Expression for a Trimer

Consider a molecular system composed of monomers A , B , and C . The total energy can be decomposed into one-, two-, and three-body contributions following the many-body expansion formalism¹ :

$$\begin{aligned} E_{ABC}^{\text{tot}} &= E_A + E_B + E_C + \varepsilon_{AB}^{(2)} + \varepsilon_{AC}^{(2)} + \varepsilon_{BC}^{(2)} + \varepsilon_{ABC}^{(3)}, \\ E_{ABC}^{\text{tot}} &= \sum_i E_i + \sum_{i \neq j} \varepsilon_{ij}^{(2)} + \varepsilon_{ABC}^{(3)}, \end{aligned} \tag{1}$$

where $i, j \in \{A, B, C\}$ and the ordering ij is chosen so that $i < j$ to avoid double counting. The two-body terms $\varepsilon_{ij}^{(2)}$ refer to the interaction energy between pairs of monomers, while the three-body term $\varepsilon_{ABC}^{(3)}$ represents the non-additive energy that arises only when all three monomers are present simultaneously. In other words, these terms correspond to the energy required to bring two or three monomers together, respectively.

The standard two-body interaction energy is defined as

$$\Delta E_{\text{int}}^{\text{st}}(ij) = \varepsilon_{ij}^{(2)} = E_{ij}^{\text{tot}} - (E_i + E_j), \tag{2}$$

and, analogously, the standard three-body interaction energy is

$$\Delta E_{\text{int}}^{\text{st}}(ijk) = \varepsilon_{ijk}^{(3)} = E_{ijk}^{\text{tot}} - (E_i + E_j + E_k). \tag{3}$$

By combining Eqs. (3) and (1), the total interaction energy of the system formed by monomers A , B , and C can be expressed in two equivalent ways:

$$\Delta E_{\text{int}}^{\text{st}} = E_{ABC}^{\text{tot}} - \sum_i E_i, \tag{4}$$

$$\Delta E_{\text{int}}^{\text{st}} = \varepsilon_{AB}^{(2)} + \varepsilon_{AC}^{(2)} + \varepsilon_{BC}^{(2)} + \varepsilon_{ABC}^{(3)}. \tag{5}$$

Equation (4) is typically used when the total cluster energy E_{ABC}^{tot} and the monomer energies E_A , E_B , and E_C are known from direct computation. Equation (5), in contrast, is more convenient when the two-body and three-body interaction energies are determined separately, for example, from potential energy surface calculations or incremental schemes. Thus, the interaction energy of the trimer system can be evaluated either from the total energy of the cluster and its monomers, or from the sum of the pairwise and three-body interaction contributions. In theory, if the “exact”

energies of the monomers and the cluster were available, the interaction energy of a two-particle system could be determined exactly using Eq. (2). In practice, however, this is not possible because all quantities are obtained through quantum-chemical approximations that depend on both the *level of theory*—such as Hartree–Fock (HF), Møller–Plesset perturbation theory (MP2), coupled-cluster theory with single, double, and perturbative triple excitations [CCSD(T)], or density functional theory (DFT)—and the chosen *basis set* used to represent the molecular orbitals.

The fundamental problem that arises is one of **basis-set inconsistency**. Within the framework of the variational principle and the Roothaan–Hall approximation,^{2,3} molecular orbitals are expressed as linear combinations of a finite set of *basis functions* (often referred to as atomic orbitals). In this context, the total basis set of the supermolecule is larger than that of the individual monomers: the supermolecule basis consists of all basis functions associated with every monomer in the system, whereas each isolated monomer is described only by its own subset of basis functions. Consequently, the total energy of the cluster is evaluated in a more complete variational space than that of the separated monomers.

If we compute the standard interaction energy of the AB cluster under these conditions, we obtain

$$\Delta E_{\text{int}}^{\text{st}} = E_{AB}^{\text{tot}}(AB) - [E_A(A) + E_B(B)], \quad (6)$$

where the notation in parentheses explicitly denotes the basis set employed for each subsystem. Because the basis used for the cluster (AB) is more extensive than that used for the isolated monomers (A) and (B), the total energy of the dimer is artificially stabilized. As a result, the corresponding interaction energy is spuriously lowered, leading to what is known as the *basis set superposition error* (BSSE).

To correct for this basis-set inconsistency, Boys and Bernardi [4] introduced the *counterpoise* (*CP*) *correction* procedure. The method was originally formulated for a two-particle system (AB), in which the total energy of the dimer AB is evaluated in the full dimer basis (AB), and each monomer energy is recomputed in the same basis while the partner monomer is replaced by *ghost* orbitals (i.e., basis functions without nuclei or electrons). The counterpoise-corrected interaction energy is then defined as

$$\Delta E_{\text{int}}^{\text{CP}} = E_{AB}^{\text{tot}}(AB) - [E_A(AB) + E_B(AB)], \quad (7)$$

where $E_A(AB)$ and $E_B(AB)$ represent the monomer energies calculated in the presence of the other monomer’s basis set.

The BSSE quantifies how much the standard interaction energy is *contaminated* by basis-set inconsistencies. A practical way to evaluate this contamination is to compute the difference between the standard (uncorrected) interaction energy and the counterpoise-corrected one⁵:

$$\text{BSSE} = \Delta E_{\text{int}}^{\text{st}} - \Delta E_{\text{int}}^{\text{CP}} = [E_A(AB) + E_B(AB)] - [E_A(A) + E_B(B)]. \quad (8)$$

Since interaction energies for bound systems are typically negative (attractive), a *negative* BSSE indicates that the uncorrected interaction energy, $\Delta E_{\text{int}}^{\text{st}}$, is *too attractive*. After applying the counterpoise correction, the resulting interaction energy $\Delta E_{\text{int}}^{\text{CP}}$ is therefore **less negative**, and thus

$$\text{BSSE} < 0.$$

This negative value represents the **fictitious stabilization**—the artificial energy lowering that arises purely from basis-set imbalance. Hence, the difference above quantifies how much of the apparent overbinding is due to BSSE.

One of the first extensions of the counterpoise (CP) correction to trimers was given by White and Davidson in their study of hydrogen-bonded ice,⁶ and later generalized by Valiron and Mayer.¹ In this framework, each two-body interaction energy $\varepsilon_{ij}^{(2)}$ ($i, j \in \{A, B, C\}$) is evaluated with CP as in Eq. (2) and assembled in Eq. (5). The remaining term, $\varepsilon_{ijk}^{(3)}$, is the *pure three-body* contribution. It is obtained from the many-body expansion for the trimer, Eq. (1), with CP applied consistently to all monomer and dimer terms:

$$\begin{aligned} \varepsilon_{ABC}^{(3)}(ABC) = E_{ABC}^{\text{tot}}(ABC) - [E_A(ABC) + E_B(ABC) + E_C(ABC) \\ + \varepsilon_{AB}^{(2)}(ABC) + \varepsilon_{AC}^{(2)}(ABC) + \varepsilon_{BC}^{(2)}(ABC)]. \end{aligned} \quad (9)$$

From here the (CP) interaction energy for the trimer can be written as

$$\Delta E_{\text{int}}^{\text{CP}} = \varepsilon_{AB}^{(2)}(AB) + \varepsilon_{AC}^{(2)}(AC) + \varepsilon_{BC}^{(2)}(BC) + \varepsilon_{ABC}^{(3)}(ABC) \quad (10)$$

which can be arranged into the following 16-term expression by considering each contribution:

$$\begin{aligned} \Delta E_{\text{int}}^{\text{CP}} = E_{AB}(AB) - [E_A(AB) + E_B(AB)] + E_{AC}(AC) - [E_A(AC) + E_C(AC)] \\ + E_{BC}(BC) - [E_B(BC) + E_C(BC)] + \mathcal{E}_{ABC} \end{aligned} \quad (11)$$

where

$$\mathcal{E}_{ABC} = E_{ABC}(ABC) - [E_{AB}(ABC) + E_{AC}(ABC) + E_{BC}(ABC) - [E_A(ABC) + E_B(ABC) + E_C(ABC)]]$$

Now, the standard interaction energy for the trimer is given by

$$\Delta E_{\text{int}}^{\text{st}} = E_{ABC}(ABC) - [E_A(A) + E_B(B) + E_C(C)] \quad (12)$$

and from here the BSSE is given by

$$\begin{aligned} \text{BSSE} &= \Delta E_{\text{int}}^{\text{st}} - \Delta E_{\text{int}}^{\text{CP}} \\ &= \left[[E_A(AB) + E_A(AC)] - [E_A(ABC) + E_A(A)] \right] \\ &\quad + \left[[E_B(AB) + E_B(BC)] - [E_B(ABC) + E_B(B)] \right] \\ &\quad + \left[[E_C(AC) + E_C(BC)] - [E_C(ABC) + E_C(C)] \right] \\ &\quad + \left[[E_{AB}(ABC) + E_{AC}(ABC)] - [E_{AB}(AB) + E_{AC}(AC)] \right] + \left[E_{BC}(ABC) - E_{BC}(BC) \right] \end{aligned} \quad (13)$$

2. BSSE for the Trimer System: Subset Representation

In the previous section we saw that the BSSE [Eq. (13)] for a trimer depends on the monomer and dimer energies evaluated in different basis sets. If we define the set $\mathcal{B} = \{A, B, C\}$ to represent the basis sets associated with each monomer, we can describe the hierarchy of energy evaluations in terms of the subsets of \mathcal{B} .

The **power set** of \mathcal{B} , denoted $\mathcal{P}_{\mathcal{B}}$, is the set of all possible subsets of \mathcal{B} :

$$\mathcal{P}_{\mathcal{B}} = \{\emptyset, \{A\}, \{B\}, \{C\}, \{A, B\}, \{A, C\}, \{B, C\}, \{A, B, C\}\}.$$

The power set contains every possible combination of the basis sets, including the empty set, and its cardinality is given by

$$|\mathcal{P}_{\mathcal{B}}| = 2^{|\mathcal{B}|} = 2^3 = 8.$$

We are interested in the subsets that contain a given element. So, for any element $X \in \mathcal{B}$, we can define the collection of all subsets that contain X as

$$\mathcal{P}_{\mathcal{B}}(X) = \{S \subseteq \mathcal{B} \mid X \in S\}.$$

For instance,

$$\mathcal{P}_{\mathcal{B}}(A) = \{\{A\}, \{A, B\}, \{A, C\}, \{A, B, C\}\}.$$

This shows that each monomer (here A) appears in four different subsets of \mathcal{B} . Then, every subset S of \mathcal{B} that contains A can be written uniquely as

$$S = \{A\} \cup T,$$

where T is any subset of $\mathcal{B} \setminus \{A\}$. Hence,

$$\mathcal{P}_{\mathcal{B}}(A) = \{ \{A\} \cup T \mid T \subseteq \mathcal{B} \setminus \{A\} \}.$$

Now, we can see that there are $2^{|\mathcal{B}|-1}$ possible subsets $T \subseteq \mathcal{B} \setminus \{A\}$, it follows that

$$|\mathcal{P}_{\mathcal{B}}(A)| = 2^{|\mathcal{B}|-1}.$$

For a trimer ($|\mathcal{B}| = 3$), we have $|\mathcal{P}_{\mathcal{B}}(A)| = 2^2 = 4$, corresponding exactly to the subsets $\{A\}$, $\{A, B\}$, $\{A, C\}$, and $\{A, B, C\}$.

In an analogous way, we can determine all subsets of \mathcal{B} that contain a specific *pair* of elements, say A and B . These subsets correspond to all basis combinations that simultaneously include both A and B , which are relevant for the evaluation of dimer energies.

We define this collection as

$$\mathcal{P}_{\mathcal{B}}(A, B) = \{ S \subseteq \mathcal{B} \mid \{A, B\} \subseteq S \}.$$

For our trimer example,

$$\mathcal{P}_{\mathcal{B}}(A, B) = \{ \{A, B\}, \{A, B, C\} \}.$$

Each dimer therefore appears in exactly two subsets of \mathcal{B} : its own dimer basis and the full trimer basis. Following the same reasoning as before, every subset S that contains both A and B can be written uniquely as

$$S = \{A, B\} \cup T,$$

where T is any subset of the remaining elements, $\mathcal{B} \setminus \{A, B\}$. Hence,

$$\mathcal{P}_{\mathcal{B}}(A, B) = \{ \{A, B\} \cup T \mid T \subseteq \mathcal{B} \setminus \{A, B\} \}.$$

Because there are $2^{|\mathcal{B}|-2}$ possible subsets $T \subseteq \mathcal{B} \setminus \{A, B\}$, the number of subsets containing both A and B is

$$|\mathcal{P}_{\mathcal{B}}(A, B)| = 2^{|\mathcal{B}|-2}.$$

For the trimer ($|\mathcal{B}| = 3$), we obtain $|\mathcal{P}_{\mathcal{B}}(A, B)| = 2^1 = 2$, corresponding to the subsets $\{A, B\}$ and $\{A, B, C\}$, as expected.

More generally, for any k -tuple of elements $\{X_1, X_2, \dots, X_k\} \subseteq \mathcal{B}$, the collection of all subsets of \mathcal{B} containing these k elements is given by

$$\mathcal{P}_{\mathcal{B}}(X_1, X_2, \dots, X_k) = \left\{ \{X_1, X_2, \dots, X_k\} \cup T \mid T \subseteq \mathcal{B} \setminus \{X_1, X_2, \dots, X_k\} \right\},$$

with cardinality

$$|\mathcal{P}_{\mathcal{B}}(X_1, X_2, \dots, X_k)| = 2^{|\mathcal{B}|-k}. \quad (14)$$

This relation shows that:

- each monomer ($k = 1$) appears in $2^{|\mathcal{B}|-1}$ subsets,
- each dimer ($k = 2$) appears in $2^{|\mathcal{B}|-2}$ subsets,
- each trimer ($k = 3$) appears in $2^{|\mathcal{B}|-3}$ subsets, and so on.

This hierarchical pattern is precisely what underlies the structure of the BSSE corrections in the Valiron–Mayer formulation of the many-body counterpoise method.

This formalism provides a clear combinatorial interpretation of the BSSE hierarchy: each monomer must be evaluated in all subsets that contain it, while each dimer appears only in the subsets that contain both of its monomers. For the trimer case ($N = 3$), each monomer energy therefore involves four basis sets (its own, two dimer bases, and the trimer basis), whereas each dimer energy appears in two (its own and the trimer basis). This subset structure offers a systematic and general framework for expressing and counting the hierarchical counterpoise corrections in any N -body cluster.

3. Computational study and Number of total computations

From the subset formalism in Sec. 2, the number of primitive energy evaluations can be expressed compactly. Let N be the number of monomers. For each fragment size k ($1 \leq k \leq N$), there are $\binom{N}{k}$ fragments, and each fragment must be evaluated in 2^{N-k} supersets (all subsets that contain it). Thus,

$$N_{\text{eval}}^{\text{all terms}}(N) = \sum_{k=1}^N \binom{N}{k} 2^{N-k}. \quad (15)$$

However, when forming the *BSSE* as the difference between the counterpoise (CP) and standard interaction energies, the N -mer total energy $E_{1\dots N}(1\dots N)$ cancels exactly. Therefore, the $k = N$ term is not required:

$$N_{\text{eval}}^{\text{BSSE}}(N) = \sum_{k=1}^{N-1} \binom{N}{k} 2^{N-k} \quad (16)$$

Recalling the binomial theorem,⁷ we have that

$$(x + y)^n = \sum_{k=0}^n \binom{n}{k} x^k y^{n-k}.$$

Thus,

$$3^n = (1 + 2)^n = \sum_{k=0}^n \binom{n}{k} 1^k 2^{n-k} = \sum_{k=0}^n \binom{n}{k} 2^{n-k}.$$

We can then re-write Eq. (16) by allowing the index k to range from 0 to N . This defines a sum with $(N + 1)$ terms, that is, two more terms than the original. These additional terms correspond to the first and last elements of the full sum and must therefore be subtracted. Hence,

$$\sum_{k=1}^{N-1} \binom{N}{k} 2^{N-k} = \sum_{k=0}^N \binom{N}{k} 2^{N-k} - (2^N + 1) = 3^N - (2^N + 1),$$

where the term 2^N corresponds to the first term ($k = 0$) and the term 1 corresponds to the last term ($k = N$). In this way, we obtain

$$N_{\text{eval}}^{\text{BSSE}}(N) = 3^N - (2^N + 1). \quad (17)$$

For the trimer case ($N = 3$), we have

$$N_{\text{eval}}^{\text{BSSE}}(3) = 3^3 - 2^3 - 1 = 27 - 8 - 1 = \boxed{18}.$$

These 18 terms consist of:

- 12 monomer-in-subset energies: each monomer appears in $2^{3-1} = 4$ subsets, giving $3 \times 4 = 12$;
- 6 dimer-in-subset energies: each dimer appears in $2^{3-2} = 2$ subsets, giving $3 \times 2 = 6$.

If, in addition, one wishes to report the *counterpoise* (CP), the trimer total energy $E_{ABC}(ABC)$ must be included:

$$N_{\text{eval}}^{\text{all terms}}(3) = 18 + 1 = \boxed{19}.$$

3.1. Geometry sampling and scaling protocol

to describe this better

Each *configuration* (geometry/scale) requires the counts above. Only the three isolated-monomer energies $E_A(A)$, $E_B(B)$, $E_C(C)$ are geometry independent and can be computed once per method/basis.

Hence, with N_{geom} geometries,

$$\begin{aligned} N_{\text{runs}}^{\text{BSSE}}(3) &= 3 + N_{\text{geom}} [18 - 3] = 3 + 15 N_{\text{geom}}, \\ N_{\text{runs}}^{\text{all terms}}(3) &= 3 + N_{\text{geom}} [19 - 3] = 3 + 16 N_{\text{geom}}. \end{aligned}$$

In the trimer study we consider four shape families: *linear*, *equilateral*, *isosceles*, and *scalene* (Fig. 1). For each family we sample 12 similar (uniformly scaled) geometries, so

to instead of 12.

$$N_{\text{geom}} = 4 \times 12 = 48.$$

Therefore,

$$\begin{aligned} N_{\text{runs}}^{\text{BSSE}}(3) &= 3 + 15 \times 48 = \mathbf{723}, \\ N_{\text{runs}}^{\text{all terms}}(3) &= 3 + 16 \times 48 = \mathbf{771}. \end{aligned}$$

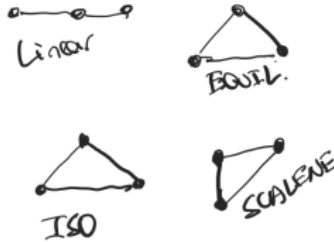


Figure 1: Trimer shape families used for scaling: linear, equilateral, isosceles, and scalene.

Electronic-structure methods and basis sets

This gives HF and MP2

All computations will be performed with three methods (HF, MP2, CCSD(T)) and two basis sets (aug-cc-pVDZ, aug-cc-pVTZ). If wall-time permits, aug-cc-pVQZ will also be included. So, for $M = 3$ (methods) and $B \in \{2, 3\}$ (basis sets). The total number of runs is

$$\begin{aligned} N_{\text{runs}}^{\text{BSSE}}(3; M, B) &= (3 + 15 N_{\text{geom}}) MB = \mathbf{723 MB}, \\ N_{\text{runs}}^{\text{all terms}}(3; M, B) &= (3 + 16 N_{\text{geom}}) MB = \mathbf{771 MB}, \end{aligned}$$

where $N_{\text{geom}} = 48$ for the four shape families with 12 scale points each.

With two basis sets ($B = 2$):

$$N_{\text{runs}}^{\text{BSSE}}(3) = 723 \times 3 \times 2 = \mathbf{4338},$$
$$N_{\text{runs}}^{\text{all terms}}(3) = 771 \times 3 \times 2 = \mathbf{4626}.$$

If aug-cc-pVQZ is added ($B = 3$):

$$N_{\text{runs}}^{\text{BSSE}}(3) = 723 \times 3 \times 3 = \mathbf{6507},$$
$$N_{\text{runs}}^{\text{all terms}}(3) = 771 \times 3 \times 3 = \mathbf{6939}.$$

4. Project file layout and NWChem job plan

To keep the workflow reproducible and scriptable, we organize all runs by molecule/method/basis/shape/scale/. Methods are HF, MP2, CCSD(T); basis sets are AVDZ (aug-cc-pVDZ), AVTZ (aug-cc-pVTZ), and optionally AVQZ.

Directory structure (per molecule).

```
<MOLECULE>/
  monomers/                                # geometry-independent monomer self-energies
    HF/
      AVDZ/  E_A(A).out  E_B(B).out  E_C(C).out
      AVTZ/  ...
      AVQZ/  ...          (optional)
    MP2/
      AVDZ/  ...
    CCSD(T)/
      AVDZ/  ...
  HF/
    AVDZ/
      linear/
        s001/  input.nw  terms.csv  logs/
        s002/  ...
        ...
      equilateral/
        s001/  ...
      isosceles/
        s001/  ...
```

One loop to go through
all files not all the
Branching

```

scalene/
  s001/    ...
  AVTZ/    (same shape/scale layout)
  AVQZ/    (optional)
  MP2/     (same per-basis, per-shape, per-scale layout)
  CCSD(T)/ (same)

```

Here `s001`, `s002`, ... are the scale values from the shape family (Sec. 3.1). Each `sXXX/` directory holds all per-geometry calculations and a summary `terms.csv`.

Canonical filenames for the 18 BSSE terms. We label energies as $E_{\text{frag}}(\text{basis})$ and encode them with underscores for file names:

`E_FRAG_BASIS.out` where $\text{FRAG} \in \{A, B, C, AB, AC, BC\}$, $\text{BASIS} \in \{A, B, C, AB, AC, BC, ABC\}$.

For a trimer geometry, compute the following files (15 per geometry if the 3 isolated monomers are reused; 18 if recomputed; the optional total trimer adds one more):

File	Meaning	Per-geom?
<code>E_A_A.out</code> , <code>E_B_B.out</code> , <code>E_C_C.out</code>	$E_A(A), E_B(B), E_C(C)$	no (compute once)
<code>E_A_AB.out</code> , <code>E_A_AC.out</code> , <code>E_A_ABC.out</code>	$E_A(AB), E_A(AC), E_A(ABC)$	yes
<code>E_B_AB.out</code> , <code>E_B_BC.out</code> , <code>E_B_ABC.out</code>	$E_B(AB), E_B(BC), E_B(ABC)$	yes
<code>E_C_AC.out</code> , <code>E_C_BC.out</code> , <code>E_C_ABC.out</code>	$E_C(AC), E_C(BC), E_C(ABC)$	yes
<code>E_AB_AB.out</code> , <code>E_AB_ABC.out</code>	$E_{AB}(AB), E_{AB}(ABC)$	yes
<code>E_AC_AC.out</code> , <code>E_AC_ABC.out</code>	$E_{AC}(AC), E_{AC}(ABC)$	yes
<code>E_BC_BC.out</code> , <code>E_BC_ABC.out</code>	$E_{BC}(BC), E_{BC}(ABC)$	yes
<i>optional:</i> <code>E_ABC_ABC.out</code>	$E_{ABC}(ABC)$	yes (needed for CP or std.)

Per-geometry summary. After all files finish in `sXXX/`, write a single row to `terms.csv`:

```

shape,scale,EA_A,EB_B,EC_C,EA_AB,EA_AC,EA_ABC,EB_AB,EB_BC,EB_ABC,
EC_AC,EC_BC,EC_ABC,EAB_AB,EAB_ABC,EAC_AC,EAC_ABC,EBC_BC,EBC_ABC,EABC_ABC

```

(Include `EABC_ABC` only if you compute CP/standard interaction energies.)

NWChem input strategy (practical notes). The implementation of the 15 per-geometry jobs can be done in either of two ways:

- (a) **One input per term** (simplest to script): write 15 small `.nw` files in `sXXX/`, each producing one `E_*.out`.
- (b) **One input that runs multiple tasks** (fewer files): reuse the same geometry and change ghost/fragment settings between `task` blocks so the output prints each energy with a clear tag.

Only the three monomer self-energies $E_A(A)$, $E_B(B)$, $E_C(C)$ are geometry independent; compute them once per method/basis under `monomers/<method>/<basis>/` and reuse across all shapes/scales.

Automation hook. I will consider a consistent JSON file alongside each `sXXX/` directory (e.g., `config.json`) containing the three Cartesian coordinates and the scale s . A python script can: (i) generate all `.nw` inputs from the JSON file, (ii) parse energies from `.out` files, (iii) append a row to `terms.csv`, and (iv) compute the BSSE difference for that geometry. This keeps the pipeline reproducible and easy to re-run for new basis sets. Note, Any recommendations are welcome!

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