

Atom- and Bond-Deletion Laplacian Response Descriptors for Molecular Graphs

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(Received April 28, 2026)

Abstract

We introduce two perturbative spectral descriptors for molecular graphs: the atom-deletion Laplacian response and the bond-deletion Laplacian response. For a hydrogen-suppressed molecular graph these quantities measure the magnitude of the change in Laplacian energy caused by deleting a single atom or a single bond. The construction is deliberately positioned relative to local Laplacian energy: it uses absolute deletion-induced variation to describe sensitivity, whereas signed local quantities retain directional increase or decrease. We cite the corresponding local Laplacian-energy results explicitly and distinguish the elementary estimates used here from sharper estimates already available in the literature. We prove a universal upper bound for the bond-deletion response of an n -vertex graph and show that it is sharp for every fixed order $n \geq 2$; we also record a transparent degree-dependent upper bound for the atom response and give exact benchmark computations for complete graphs and star graphs. On the chemical side, we analyse six representative octane isomer skeletons and then screen the full set of all 18 hydrogen-suppressed octane skeletons. A comparison with Wiener, Randić,

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Zagreb, and ordinary Laplacian-energy descriptors shows that the new totals $\mathcal{A}$ and $\mathcal{B}$, like ordinary Laplacian energy, distinguish all 18 octane skeletons while also providing local deletion-response profiles. A preliminary six-isomer boiling-point test, based on standard NIST values, confirms chemically sensible ordering but does not justify replacing the strongest classical indices on such a small sample. The paper therefore contributes a mathematically explicit sensitivity-descriptor family with preliminary chemical discrimination rather than a completed quantitative structure-property relationship model.

1 Introduction

Topological descriptors derived from molecular graphs remain central in mathematical chemistry because they connect structural information with chemical behaviour in a form that can be analysed rigorously and, in favourable cases, incorporated into quantitative structure-property relationship (QSPR)/quantitative structure-activity relationship (QSAR) models. Classical examples include the Wiener index, the Randić connectivity index, and many later degree-based, distance-based, and spectral descriptors [14, 16–18]. Their success also illustrates a broader principle: no single invariant captures every chemically relevant structural feature, so new descriptors are worthwhile when they isolate a genuinely different aspect of molecular organisation. Recent overviews of modern chemical graph theory also emphasise that useful descriptor design increasingly benefits from controlled graph perturbations, multiscale encoding, and explicit interpretability rather than from static counting alone [10].

One increasingly important theme is the construction of *response descriptors*. Instead of summarising a molecular graph only in its unperturbed state, such descriptors quantify how a graph reacts to a prescribed local modification. This viewpoint is particularly natural in mathematical chemistry, because atoms and bonds are not merely combinatorial objects; they are sites at which local structural changes can propagate through the entire molecular skeleton. In that sense, response descriptors complement recent chemically oriented topological-index developments by encoding not only structure but also the sensitivity of structure under a prescribed local perturbation [1, 6, 15].

Let G be a finite simple graph with vertex set $V(G) = \{v_1, \dots, v_n\}$, edge set $E(G)$, order n , size m , Laplacian matrix $L(G)$, and Laplacian eigenvalues

$$\mu_1 \geq \mu_2 \geq \dots \geq \mu_n.$$

Following the graph-energy tradition initiated by Gutman [7] and the Laplacian-energy definition of Gutman and Zhou [9], the Laplacian energy of G is defined by

$$\text{LE}(G) = \sum_{k=1}^n \left| \mu_k - \frac{2m}{n} \right|.$$

This invariant has been studied from several directions in graph theory and chemical graph theory, particularly because it combines spectral and size information in a tractable way [9, 13].

Recent work has shown that deletion operations provide a useful local perspective on graph energies. Day and So studied energy change under edge deletion [3, 4]; Allem, Jacobs and Trevisan investigated analogous questions for normalized Laplacian energy [2]; Espinal and Rada studied graph energy change under vertex deletion [5]; and Moon and Park introduced local Laplacian energy under vertex deletion [13]. The present manuscript is closely connected with this line of work, especially with the local Laplacian-energy framework of Moon and Park. We therefore use their paper as the main reference point when discussing vertex deletion: the spectral lemma below is a restatement of their two-eigenvalue computation in the notation needed here, and the degree-dependent atom-deletion estimate is an elementary bound rather than an improvement over their sharper trace-norm estimate. The new descriptor-oriented component is the use of absolute deletion responses as molecular sensitivity profiles, together with the parallel treatment of atom deletion and bond deletion in a chemical graph setting.

In a hydrogen-suppressed molecular graph, deleting a vertex may be interpreted as deleting a heavy atom from the molecular skeleton, while deleting an edge corresponds to deleting a bond. This motivates the present paper. We study the *absolute* change in Laplacian energy caused by a single atom deletion or bond deletion and treat the resulting quantities as

local chemical-sensitivity descriptors.

The specific contribution of the paper lies in four points.

- (i) We formulate atom-deletion and bond-deletion Laplacian *response* descriptors tailored to molecular graphs and explicitly distinguish them from signed local Laplacian-energy quantities.
- (ii) We record an elementary degree-dependent upper bound for the atom response, while acknowledging that the sharper local Laplacian-energy estimate of Moon and Park gives the stronger inequality in the corresponding vertex-deletion setting.
- (iii) We prove a universal upper bound for the bond-deletion response that is sharp for every fixed order $n \geq 2$ and give exact benchmark computations for complete graphs and star graphs; the star calculation is presented as an illustrative example because its vertex-deletion part follows directly from known local Laplacian-energy formulas.
- (iv) We show on octane, nonane, and decane skeletons that the descriptor pair $(\mathcal{A}, \mathcal{B})$ gives interpretable structural discrimination and local deletion-response profiles.

The present contribution is best viewed as a descriptor-development study rather than as a finished QSPR/QSAR model. Its main value lies in the mathematically explicit introduction and analysis of a response-based Laplacian-energy descriptor family. The octane-isomer section is included as a chemically interpretable first case study, and the exhaustive screen over all 18 octane skeletons is intended to test the structural discriminating power of the descriptors without overstating the work as a completed property-prediction study.

The paper is organised as follows. Section 2 collects notation and basic tools. Section 3 studies atom-deletion response. Section 4 treats bond-deletion response. Section 5 provides exact benchmark families. Section 6 contains the octane-isomer case study. Section 7 compares the new descriptors with standard indices and includes a preliminary boiling-point test. Section 8 discusses novelty, chemical relevance, and current limitations. Section 9 closes the paper.

2 Preliminaries

For a graph G , let $A(G)$ be its adjacency matrix and let $D(G)$ be the diagonal degree matrix. The Laplacian matrix is

$$L(G) = D(G) - A(G).$$

If d_k denotes the degree of v_k , then the average degree is

$$\bar{d} = \frac{1}{n} \sum_{k=1}^n d_k = \frac{2m}{n}.$$

Since $L(G)$ is symmetric,

$$\text{LE}(G) = \|L(G) - \bar{d}I_n\|_*,$$

where $\|\cdot\|_*$ denotes the trace norm (nuclear norm), that is, the sum of singular values.

We shall repeatedly use the standard estimate

$$|\|X\|_* - \|Y\|_*| \leq \|X - Y\|_* \tag{1}$$

valid for all real matrices X, Y of the same size; see, for example, standard trace-norm triangle-equality discussions such as [11].

The following spectral lemma is the main local computation used later. It is included to fix notation, but the result is not new: the same matrix reduction and the same two nontrivial eigenvalues appear in Lemma 2 of Moon and Park [13] in their study of local Laplacian energy.

Lemma 1. *Let $n \geq 2$ and $k \in \mathbb{R}$, and let*

$$M_n(k) = \begin{bmatrix} k & -1 & -1 & \cdots & -1 \\ -1 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ -1 & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Then the spectrum of $M_n(k)$ is

$$\text{Spec}(M_n(k)) = \left\{ 1^{(n-2)}, \frac{k+1 - \sqrt{(k-1)^2 + 4(n-1)}}{2}, \frac{k+1 + \sqrt{(k-1)^2 + 4(n-1)}}{2} \right\}.$$

Proof. The vectors $x = (0, x_2, \dots, x_n)^T$ satisfying $\sum_{i=2}^n x_i = 0$ form an $(n-2)$ -dimensional subspace, and each satisfies $M_n(k)x = x$. Thus 1 has multiplicity $n-2$. The complementary invariant subspace is spanned by e_1 and $s = e_2 + \dots + e_n$. In the basis $\{e_1, s\}$, the restriction has matrix

$$\begin{bmatrix} k & -(n-1) \\ -1 & 1 \end{bmatrix}.$$

Its characteristic polynomial is

$$\lambda^2 - (k+1)\lambda + k - (n-1),$$

which gives the two displayed roots. Together with the $n-2$ copies of 1, these account for all eigenvalues. ■

We now introduce the new descriptors.

Definition 1. Let G be a graph.

- (a) For $v \in V(G)$, the *atom-deletion Laplacian response* of G at v is

$$\alpha_G(v) = |\text{LE}(G) - \text{LE}(G-v)|.$$

The *total atom response* is

$$\mathcal{A}(G) = \sum_{v \in V(G)} \alpha_G(v).$$

(b) For $e \in E(G)$, the *bond-deletion Laplacian response* of G at e is

$$\beta_G(e) = |\text{LE}(G) - \text{LE}(G - e)|.$$

The *total bond response* is

$$\mathcal{B}(G) = \sum_{e \in E(G)} \beta_G(e).$$

Remark. For molecular graphs these descriptors are perturbative rather than static. The quantity $\alpha_G(v)$ measures how strongly the Laplacian energy reacts to deleting atom v , whereas $\beta_G(e)$ measures the analogous response to deleting bond e . The functions $v \mapsto \alpha_G(v)$ and $e \mapsto \beta_G(e)$ therefore provide local response profiles in addition to the global totals $\mathcal{A}(G)$ and $\mathcal{B}(G)$.

Remark (signed variation versus absolute response). It is useful to distinguish the present response descriptors from the signed local quantities

$$\ell_G(v) = \text{LE}(G) - \text{LE}(G - v), \quad b_G(e) = \text{LE}(G) - \text{LE}(G - e).$$

Their sums,

$$\ell(G) = \sum_{v \in V(G)} \ell_G(v), \quad b(G) = \sum_{e \in E(G)} b_G(e),$$

retain directional information: a positive value means that deletion decreases Laplacian energy, while a negative value means that deletion increases it. By contrast, $\mathcal{A}(G)$ and $\mathcal{B}(G)$ measure the total magnitude of the perturbation. This absolute-value formulation is therefore a sensitivity descriptor. It prevents cancellation when positive and negative signed changes coexist and gives naturally nonnegative atom- and bond-level profiles. The price is that the direction of change is no longer visible from the total alone; for this reason the signed quantities remain useful complementary diagnostics. In the chemical computations below we report the absolute responses as the proposed descriptors and discuss explicitly where signed cancellation is or is not relevant.

3 Atom-deletion Laplacian response

Let G be a graph of order n and size m , let $v \in V(G)$, and let d_v be the degree of v . We write

$$\bar{d} = \frac{2m}{n}, \quad \bar{d}^{(v)} = \frac{2(m - d_v)}{n - 1},$$

where $\bar{d}^{(v)}$ is the average degree of $G - v$.

The next result gives an elementary atom-response estimate. It is retained because it is short, transparent, and directly tied to the response descriptor, not because it improves the sharper local Laplacian-energy bound of Moon and Park [13].

Theorem 1. *Let G be a graph of order $n \geq 2$ and size m , and let $v \in V(G)$ have degree d_v . Put*

$$\bar{d} = \frac{2m}{n}, \quad \bar{d}^{(v)} = \frac{2(m - d_v)}{n - 1}.$$

Then

$$\alpha_G(v) \leq 2d_v + \bar{d} + (n - 1) \left| \bar{d}^{(v)} - \bar{d} \right|.$$

Equivalently,

$$\alpha_G(v) \leq 2d_v + \frac{2m}{n} + \frac{2|m - nd_v|}{n}.$$

Proof. Let

$$X = L(G) - \bar{d}I_n$$

and let $X^{(v)} = L(G - v) - \bar{d}^{(v)}I_{n-1}$. Embed $X^{(v)}$ into an $n \times n$ matrix $Y^{(v)}$ by inserting a zero row and a zero column at the position corresponding to v . Since the insertion adds only a zero singular value,

$$\alpha_G(v) = \left| \|X\|_* - \|Y^{(v)}\|_* \right| \leq \|X - Y^{(v)}\|_*$$

by the reverse triangle inequality for the trace norm.

Let B_v denote the Laplacian matrix of the star formed by the vertex v and its d_v neighbours, embedded in the full vertex set of G and zero outside this vertex-neighbourhood block. If $d_v = 0$, then $B_v = 0$ and the

same estimate below is immediate. Hence assume $d_v \geq 1$. Then

$$X - Y^{(v)} = B_v - \bar{d}E_{vv} + (\bar{d}^{(v)} - \bar{d})(I_n - E_{vv}),$$

where E_{vv} is the matrix with a single 1 in the (v, v) position and zeros elsewhere. By Lemma 1, applied to the embedded star block of size $d_v + 1$ with $k = d_v$, the non-zero Laplacian eigenvalues of this embedded star are $d_v + 1$ and 1 with multiplicity $d_v - 1$, so

$$\|B_v\|_* = (d_v + 1) + (d_v - 1) = 2d_v.$$

The two diagonal perturbation terms have trace norms $\bar{d}$ and $(n-1)|\bar{d}^{(v)} - \bar{d}|$, respectively. Therefore

$$\|X - Y^{(v)}\|_* \leq 2d_v + \bar{d} + (n-1)|\bar{d}^{(v)} - \bar{d}|.$$

The displayed equivalent form follows from

$$\bar{d}^{(v)} - \bar{d} = \frac{2(m - nd_v)}{n(n-1)}.$$

This completes the proof. ■

Corollary 2. *Let G be a graph of order n and size m . Then*

$$\mathcal{A}(G) \leq \sum_{v \in V(G)} \left(2d_v + \frac{2m}{n} + \frac{2|m - nd_v|}{n} \right).$$

In particular,

$$\mathcal{A}(G) \leq 12m.$$

Proof. The first inequality follows by summing Theorem 1. For the displayed uniform bound, use $|m - nd_v| \leq m + nd_v$ and $\sum_{v \in V(G)} d_v = 2m$. Hence

$$\sum_{v \in V(G)} \frac{2|m - nd_v|}{n} \leq \frac{2}{n} \sum_{v \in V(G)} (m + nd_v) = 6m.$$

Together with $\sum_v 2d_v = 4m$ and $\sum_v 2m/n = 2m$, this gives $\mathcal{A}(G) \leq 12m$. ■

Corollary 3. *If T is a molecular tree of order $n \geq 2$ and maximum degree at most 4, then*

$$\mathcal{A}(T) \leq 8(n-1).$$

More precisely,

$$\mathcal{A}(T) \leq \sum_{v \in V(T)} \left(2d_v + \frac{2(n-1)}{n} + \frac{2|n-1-nd_v|}{n} \right).$$

Proof. Since T is a tree, $m = n - 1$ and $\sum_v d_v = 2(n - 1)$. Also every vertex of a connected tree with $n \geq 2$ has $d_v \geq 1$, and therefore

$$|n - 1 - nd_v| = nd_v - n + 1.$$

Substituting this into the more precise estimate gives, for each vertex v ,

$$2d_v + \frac{2(n-1)}{n} + \frac{2(nd_v - n + 1)}{n} = 4d_v.$$

Summing over all vertices yields $\mathcal{A}(T) \leq 4 \sum_v d_v = 8(n - 1)$. ■

Remark (comparison with the sharper local estimate). The estimate in Theorem 1 is intentionally stated in a form that is valid for all finite simple graphs and whose proof uses only the trace-norm triangle inequality and the exact spectrum of an embedded star. It is not claimed to be sharp in general. In fact, Moon and Park [13] obtained the sharper local Laplacian-energy estimate

$$\begin{aligned} |\text{LE}(G) - \text{LE}(G - v)| &\leq (n - d_v - 1) \left| \bar{d}^{(v)} - \bar{d} \right| + (d_v - 1) \left| 1 + \bar{d}^{(v)} - \bar{d} \right| \\ &\quad + \sqrt{(d_v - \bar{d}^{(v)} - 1)^2 + 4d_v}. \end{aligned}$$

This sharper estimate can be exact. For example, for the star S_6 and its center vertex v , Theorem 1 gives the non-sharp value 20, whereas the Moon–Park bound gives $26/3$, which equals the exact value of $\text{LE}(S_6)$. Thus Theorem 1 should be read only as an elementary universal response estimate. The numerical section computes the exact responses directly from Laplacian spectra rather than from this upper bound.

4 Bond-deletion Laplacian response

We now turn to bond deletion. This case is particularly natural in mathematical chemistry because it quantifies the spectral response of a molecular skeleton to the removal of a single bond.

Theorem 4. *Let G be a graph of order n and let $e \in E(G)$. Then*

$$\beta_G(e) \leq 4 - \frac{4}{n}.$$

This bound is sharp.

Proof. Let $e = uv$. Write

$$X = L(G) - \bar{d}I_n, \quad X_e = L(G - e) - \bar{d}_e I_n,$$

where $\bar{d} = 2m/n$ and $\bar{d}_e = 2(m-1)/n = \bar{d} - 2/n$. Then by (1),

$$\beta_G(e) = \left| \|X\|_* - \|X_e\|_* \right| \leq \|X - X_e\|_*.$$

Now $L(G) - L(G - e)$ is the rank-two Laplacian contribution of the single edge uv , namely the matrix B_e having the 2×2 block

$$\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

in the rows and columns indexed by u, v , and zeros elsewhere. Thus

$$X - X_e = B_e - \frac{2}{n}I_n.$$

The matrix B_e has eigenvalues $2, 0, \dots, 0$. Therefore $X - X_e$ has eigenvalues

$$2 - \frac{2}{n}, \quad -\frac{2}{n} \text{ (with multiplicity } n-1 \text{)}.$$

Hence

$$\|X - X_e\|_* = \left| 2 - \frac{2}{n} \right| + (n-1)\frac{2}{n} = 4 - \frac{4}{n}.$$

This proves the inequality. To prove sharpness for every fixed order $n \geq 2$,

take

$$G = K_2 \cup (n-2)K_1,$$

and let e be the unique edge in the K_2 component. Then $G - e = nK_1$, so $\text{LE}(G - e) = 0$. Since G has order n and size 1, its Laplacian spectrum is $2, 0, \dots, 0$, and therefore

$$\text{LE}(G) = \left| 2 - \frac{2}{n} \right| + (n-1)\frac{2}{n} = 4 - \frac{4}{n}.$$

Thus $\beta_G(e) = 4 - 4/n$, and the bound is sharp for each admissible order. ■

An immediate consequence is the following global estimate.

Corollary 5. *If G is a graph of order n and size m , then*

$$\mathcal{B}(G) \leq m \left(4 - \frac{4}{n} \right).$$

Proof. Sum the estimate of Theorem 4 over all edges of G . ■

5 Exact benchmark families

To calibrate the new descriptors, it is useful to examine two extremal but chemically interpretable graph families: complete graphs as dense benchmarks and stars as highly branched trees.

Proposition 6. *For the complete graph K_n ($n \geq 2$),*

$$\begin{aligned} \text{LE}(K_n) &= 2(n-1), \\ \alpha_{K_n}(v) &= 2 \quad \text{for every } v \in V(K_n), \\ \mathcal{A}(K_n) &= 2n. \end{aligned}$$

Moreover, for every edge $e \in E(K_n)$,

$$\beta_{K_n}(e) = \left| \frac{8}{n} - 2 \right|, \quad \mathcal{B}(K_n) = \binom{n}{2} \left| \frac{8}{n} - 2 \right|.$$

Proof. The Laplacian spectrum of K_n is $\{n^{(n-1)}, 0\}$, so

$$\text{LE}(K_n) = (n-1)|n - (n-1)| + |0 - (n-1)| = 2(n-1).$$

Since $K_n - v \cong K_{n-1}$, we have

$$\alpha_{K_n}(v) = \text{LE}(K_n) - \text{LE}(K_{n-1}) = 2(n-1) - 2(n-2) = 2.$$

Thus $\mathcal{A}(K_n) = 2n$.

Now fix an edge $e = uv$. In $K_n - e$, the all-ones vector gives eigenvalue 0, the vector $\mathbf{e}_u - \mathbf{e}_v$ gives eigenvalue $n-2$, and every vector orthogonal to $\mathbf{1}$ with equal coordinates in the positions u and v gives eigenvalue n . Hence the Laplacian spectrum of $K_n - e$ is $\{n^{(n-2)}, n-2, 0\}$. Its average degree is

$$\frac{2}{n} \left(\binom{n}{2} - 1 \right) = n-1 - \frac{2}{n}.$$

Therefore

$$\begin{aligned} \text{LE}(K_n - e) &= (n-2) \left| 1 + \frac{2}{n} \right| + \left| \frac{2}{n} - 1 \right| + \left| 1 - n + \frac{2}{n} \right| \\ &= (n-2) \left(1 + \frac{2}{n} \right) + \left| \frac{2}{n} - 1 \right| + \left(n-1 - \frac{2}{n} \right). \end{aligned}$$

A simple simplification yields

$$\text{LE}(K_n - e) = 2n - \frac{8}{n}.$$

Hence

$$\beta_{K_n}(e) = \left| 2(n-1) - \left(2n - \frac{8}{n} \right) \right| = \left| \frac{8}{n} - 2 \right|.$$

Summing over all $\binom{n}{2}$ edges gives the stated formula for $\mathcal{B}(K_n)$. ■

Example 1 (star graphs). Let $S_n = K_{1,n-1}$ ($n \geq 3$), let c be its center, and let x be any leaf. The following direct computation records the response descriptors for the highly branched benchmark family:

$$\text{LE}(S_n) = 2n - 4 + \frac{4}{n}.$$

Furthermore,

$$\alpha_{S_n}(c) = 2n - 4 + \frac{4}{n}, \quad \alpha_{S_n}(x) = 2 - \frac{4}{n(n-1)}, \quad \beta_{S_n}(e) = 2 - \frac{4}{n}$$

for every edge e of S_n . Consequently,

$$\mathcal{A}(S_n) = 4n - 6, \quad \mathcal{B}(S_n) = 2n - 6 + \frac{4}{n}.$$

Proof. The Laplacian spectrum of S_n is $\{n, 1^{(n-2)}, 0\}$, while its average degree is $2(n-1)/n$. Hence

$$\begin{aligned} \text{LE}(S_n) &= \left| n - \frac{2(n-1)}{n} \right| + (n-2) \left| 1 - \frac{2(n-1)}{n} \right| + \left| 0 - \frac{2(n-1)}{n} \right| \\ &= \left(n - 2 + \frac{2}{n} \right) + (n-2) \left(1 - \frac{2}{n} \right) + \left(2 - \frac{2}{n} \right) = 2n - 4 + \frac{4}{n}. \end{aligned}$$

The vertex-deletion part is a direct evaluation of the local Laplacian-energy formulas for stars discussed by Moon and Park [13]; it is included here as an example because it calibrates the absolute-response notation. Deleting the center produces $(n-1)K_1$, so

$$\alpha_{S_n}(c) = \text{LE}(S_n) = 2n - 4 + \frac{4}{n}.$$

Deleting a leaf produces S_{n-1} , hence

$$\begin{aligned} \alpha_{S_n}(x) &= \text{LE}(S_n) - \text{LE}(S_{n-1}) \\ &= \left(2n - 4 + \frac{4}{n} \right) - \left(2n - 6 + \frac{4}{n-1} \right) \\ &= 2 - \frac{4}{n(n-1)}. \end{aligned}$$

Now let e be an edge of S_n . Then $S_n - e \cong S_{n-1} \cup K_1$. This graph has Laplacian spectrum $\{n-1, 1^{(n-3)}, 0^{(2)}\}$ and average degree $2(n-2)/n$. Therefore

$$\text{LE}(S_n - e) = \left| n - 3 + \frac{4}{n} \right| + (n-3) \left| -1 + \frac{4}{n} \right|$$

$$\begin{aligned}
& + 2 \left| -2 + \frac{4}{n} \right| \\
& = 2n - 6 + \frac{8}{n}.
\end{aligned}$$

Consequently,

$$\begin{aligned}
\beta_{S_n}(e) &= \text{LE}(S_n) - \text{LE}(S_n - e) \\
&= \left(2n - 4 + \frac{4}{n} \right) - \left(2n - 6 + \frac{8}{n} \right) \\
&= 2 - \frac{4}{n}.
\end{aligned}$$

Finally,

$$\begin{aligned}
\mathcal{A}(S_n) &= \alpha_{S_n}(c) + (n-1)\alpha_{S_n}(x) \\
&= \left(2n - 4 + \frac{4}{n} \right) + (n-1) \left(2 - \frac{4}{n(n-1)} \right) \\
&= 4n - 6,
\end{aligned}$$

and

$$\mathcal{B}(S_n) = (n-1) \left(2 - \frac{4}{n} \right) = 2n - 6 + \frac{4}{n}.$$

This completes the proof. ■

Remark. The two benchmark families reveal complementary perturbative regimes. In complete graphs the bond-response total is dominant and grows quadratically, reflecting the high redundancy of dense connectivity. In stars the central atom controls the atom-response profile, which matches the chemical intuition that a branching centre behaves as a local spectral hub.

Figure 1 visualises the exact benchmark formulas from Proposition 6 and Example 1. The figure provides a useful calibration diagram for the growth scales of $\mathcal{A}$ and $\mathcal{B}$.

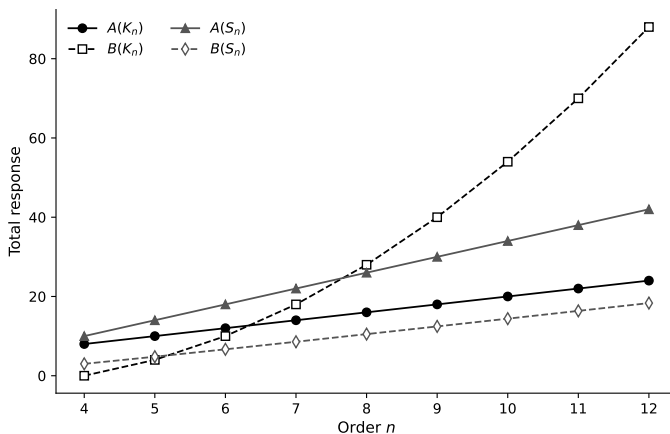


Figure 1. Benchmark behaviour of $\mathcal{A}$ and $\mathcal{B}$ for complete graphs and stars.

6 Octane isomer case study

In saturated acyclic hydrocarbons, the hydrogen-suppressed molecular graph is a tree with maximum degree at most 4. For this reason alkane skeletons provide a natural first testing ground for the descriptors introduced above.

We first consider six representative octane isomer graphs: n -octane, 2-methylheptane, 3-methylheptane, 2,2-dimethylhexane, 2,3-dimethylhexane, and 2,2,4-trimethylpentane (isooctane). Each graph has $n = 8$ vertices and $m = 7$ edges, so differences among the descriptors are caused only by branching pattern and positional arrangement. Figure 2 displays these six hydrogen-suppressed molecular graphs with vertex labels used for computation and grayscale node shading indicating degree. After this representative discussion, we extend the computation to the full family of all 18 hydrogen-suppressed octane skeletons.

6.1 Computed descriptor values

Table 1 lists the Laplacian energy, total atom response, total bond response, maximal atom response, and maximal bond response for the six octane

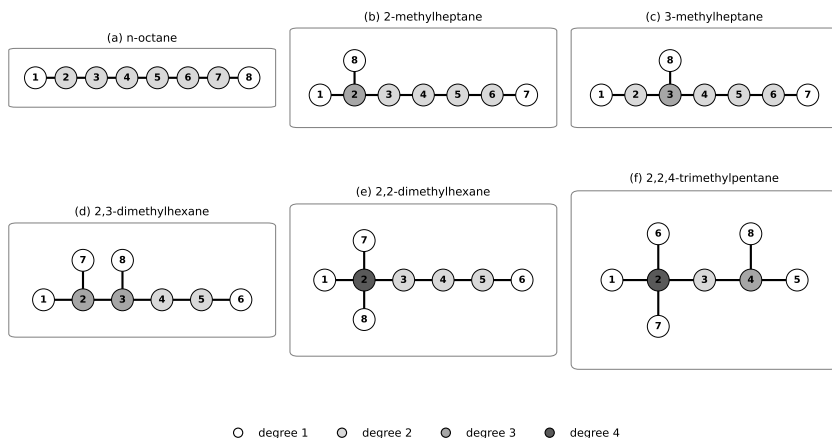


Figure 2. Hydrogen-suppressed molecular graphs of the six octane isomers used in the case study. Panel labels are included for convenient reference, vertex labels are computational indices, and grayscale node shading indicates degree.

skeletons. The values were recomputed directly from the Laplacian spectra of the corresponding graphs.

Table 1. Laplacian-energy response descriptors for representative octane skeletons; TMP denotes trimethylpentane.

Isomer	Degree sequence	LE	$\mathcal{A}$	$\mathcal{B}$	$\max \alpha$	$\max \beta$
<i>n</i> -octane	(2, 2, 2, 2, 2, 1, 1)	10.0547	12.9323	2.8304	2.1540	0.5906
2-methylheptane	(3, 2, 2, 2, 1, 1, 1)	10.4408	14.7672	3.8661	2.1838	1.0122
3-methylheptane	(3, 2, 2, 2, 2, 1, 1)	10.4556	13.7670	3.3887	2.4844	0.9915
2, 3-dimethylhexane	(3, 3, 2, 2, 1, 1, 1)	11.0583	17.6245	5.4730	3.6297	1.5861
2, 2-dimethylhexane	(4, 2, 2, 2, 1, 1, 1)	11.0955	18.1184	5.7372	3.6956	1.2671
2, 2, 4-TMP	(4, 3, 2, 1, 1, 1, 1)	11.2498	19.6956	6.5025	4.3926	1.2498

The aggregate trend is displayed in the bar chart of Figure 3. This complementary visualisation makes the ranking immediate and shows that the increase in total atom response is steeper than the increase in total bond response as branching becomes more pronounced.

Several observations follow directly from Table 1.

- (i) The linear skeleton *n*-octane has the smallest values of LE, $\mathcal{A}$, and $\mathcal{B}$ among the six examples.
- (ii) Progressive branching increases both total response descriptors. In

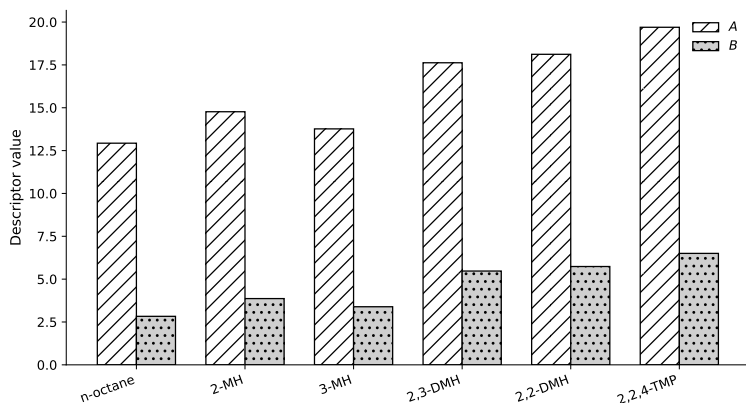


Figure 3. Comparison of the total atom and bond responses for the six octane isomers.

particular, the highly branched isooctane skeleton has the largest $\mathcal{A}$ and $\mathcal{B}$ in the sample.

- (iii) The maximal atom response grows faster than the maximal bond response, indicating that branching centres are more singular under atom deletion than any individual bond is under bond deletion.
- (iv) The descriptors distinguish positional isomers with the same degree sequence. In particular, 2-methylheptane and 3-methylheptane, as well as 2,2- and 2,3-dimethylhexane, have different response totals.

These features are important because degree sequence alone cannot separate all such examples. The pair $(\mathcal{A}, \mathcal{B})$ therefore encodes more information than a purely degree-based summary while remaining easy to interpret locally.

6.2 Local response profiles

To highlight the local structure more clearly, Table 2 compares the atom-response profiles of the linear octane chain and isooctane. In the chain, the response is distributed comparatively smoothly along the interior vertices.

In isooctane, the quaternary carbon and its neighbouring tertiary site dominate the profile.

Table 2. Atom-response profiles for *n*-octane and 2, 2, 4-trimethylpentane.

Molecule	Vertex label	Degree	$\alpha_G(v)$
<i>n</i> -octane	3	2	2.1540
	6	2	2.1540
	4	2	1.7977
	5	2	1.7977
	2	2	1.1620
	7	2	1.1620
	1	1	1.3525
	8	1	1.3525
2, 2, 4-trimethylpentane	2	4	4.3926
	4	3	3.5355
	3	2	2.9641
	1	1	1.8144
	6	1	1.8144
	7	1	1.8144
	5	1	1.6801
	8	1	1.6801

The global trend is summarised in Figure 5, which plots the six octane isomers in the $(\mathcal{A}, \mathcal{B})$ plane. The arrangement is close to monotone with branching intensity, while the separation between 2-methylheptane and 3-methylheptane shows that the response pair captures positional information beyond coarse branching count.

Figure 4 compares the indexed atom-response profiles for the linear skeleton *n*-octane and the branched isooctane skeleton 2, 2, 4-trimethylpentane. The contrast highlights how strongly the quaternary centre reorganises the local perturbation pattern in the branched molecule.

The octane data should be interpreted as a structurally transparent first illustration rather than as a complete validation study. Even so, they already show that the descriptors are responsive to both branching intensity and branching position, which is exactly the type of behaviour one would

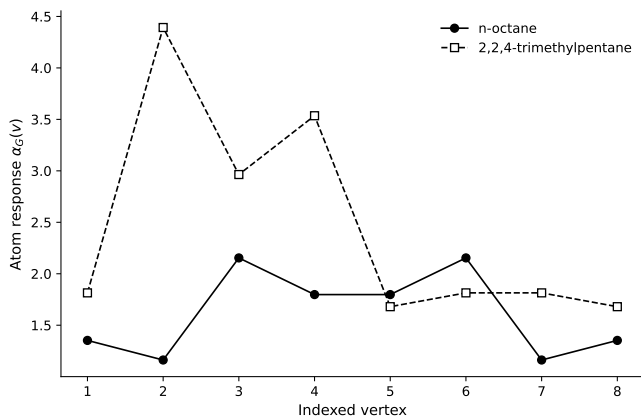


Figure 4. Comparison of atom-response profiles for *n*-octane and 2,2,4-trimethylpentane.

want from a new molecular graph descriptor.

6.3 Exhaustive screen over all octane skeletons

The representative six-isomer discussion can be strengthened by removing the element of selection. Graph-theoretically, hydrogen-suppressed octane skeletons are exactly the nonisomorphic trees on 8 vertices with maximum degree at most 4. There are 18 such trees, corresponding to the full constitutional-isomer family of octane. We generated and evaluated all 18 of them using the same Laplacian-spectral computation as in the representative study.

Figure 6 shows the entire family, indexed as $O_1, \dots, O_{18}$ in increasing order of $\mathcal{A}$ (with $\mathcal{B}$ used as a tie-breaker). The complete numerical values are reported in Appendix B. Figure 7 plots the full family in the $(\mathcal{A}, \mathcal{B})$ plane; the six representative isomers discussed earlier are highlighted.

The exhaustive screen sharpens several conclusions.

- (i) The linear chain O_1 (*n*-octane) is the unique minimum for both $\mathcal{A}$ and $\mathcal{B}$, whereas the maximally compact skeleton O_{18} (2,2,3,3-tetramethylbutane) is the unique maximum for both totals.
- (ii) Degree sequence alone is insufficient throughout the family. For

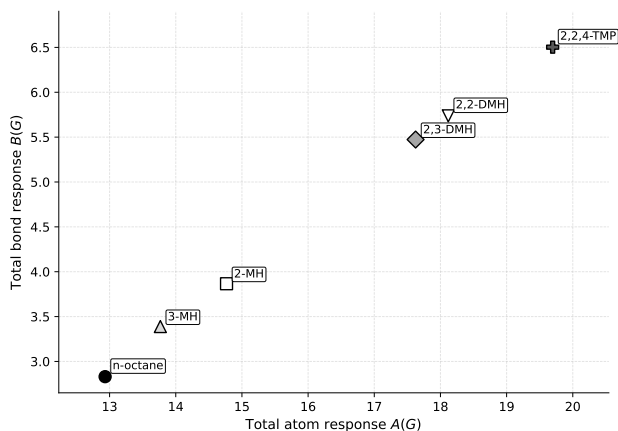


Figure 5. Response map of the six octane isomers in the (A, B) plane.

example, the four isomers with degree sequence $(3, 2, 2, 2, 2, 1, 1, 1)$ occupy different points in the response map, and the several families with degree sequence $(3, 3, 2, 2, 1, 1, 1, 1)$ are also clearly separated.

- (iii) The exhaustive data support the earlier chemical interpretation: increasing branching tends to push the family upward and to the right in the response map, but positional arrangement still creates visible secondary separation inside the same coarse branching class.

For a descriptor-development paper this exhaustive octane-family calculation is useful because it demonstrates that the response pattern is not an artefact of six hand-picked examples. Rather, the same structural trend persists across the entire constitutional family at fixed molecular formula.

6.4 Additional structural validation on nonane and decane skeletons

To avoid drawing conclusions from octane alone, we also screened the nonisomorphic hydrogen-suppressed skeletons of nonane and decane, again restricting to trees of maximum degree at most 4. Table 3 reports the number of distinct values obtained by several descriptors after rounding numerical values to 10^{-10} . No collisions were observed for the response

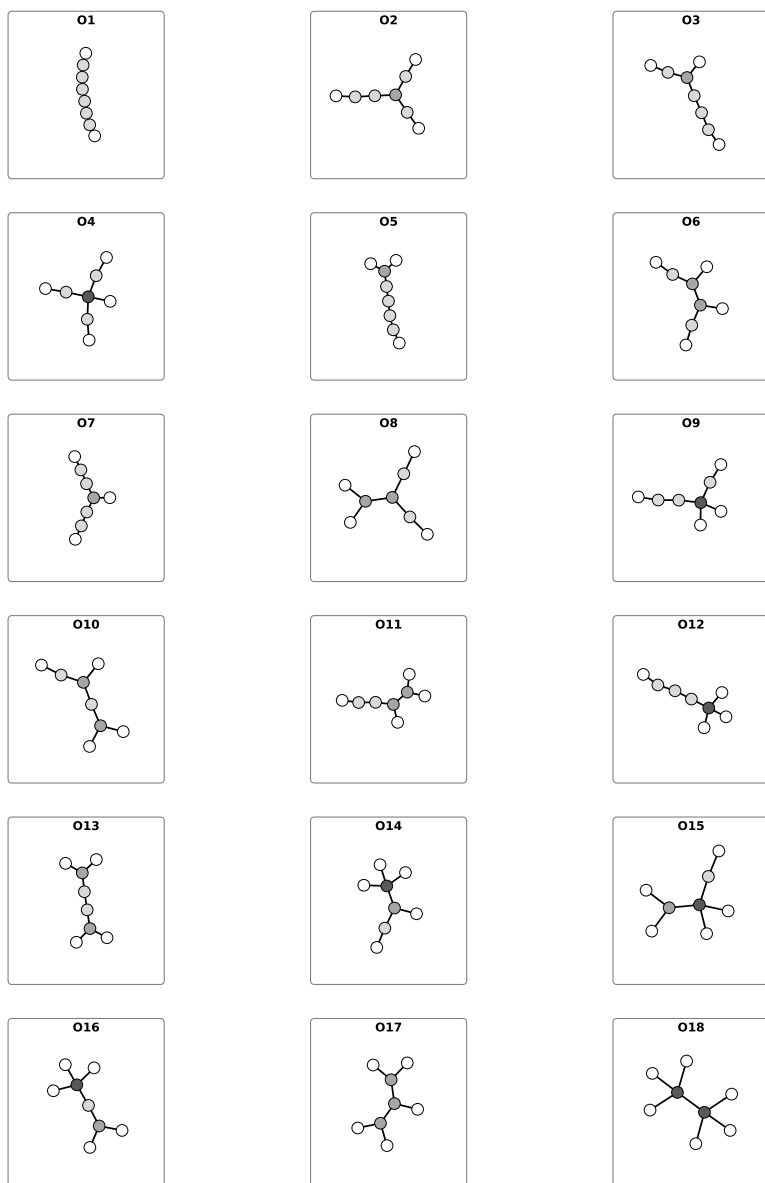


Figure 6. All 18 hydrogen-suppressed octane skeletons, indexed as $O_1, \dots, O_{18}$ by increasing total atom response $\mathcal{A}$. Only labels are shown in the panels; full names corresponding to the labels are listed in Appendix B.

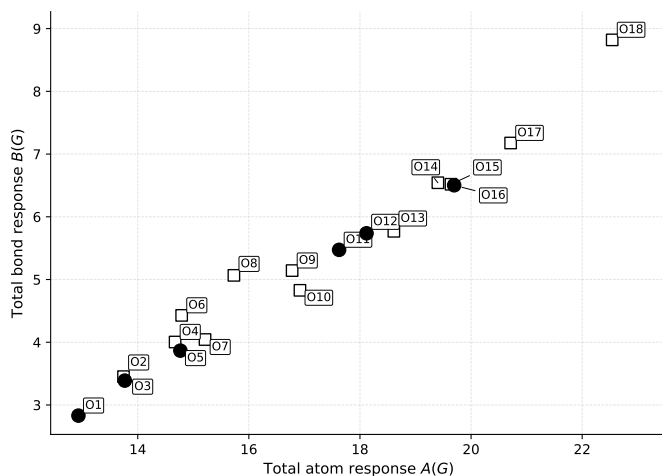


Figure 7. Response map of all 18 octane skeletons in the $(\mathcal{A}, \mathcal{B})$ plane. Filled markers indicate the six representative isomers analysed earlier in detail, while open markers denote the remaining members of the family. Labels are offset to avoid overlap.

totals on the C_9 and C_{10} alkane-skeleton families under this numerical criterion, whereas the selected classical descriptors have repeated values. This computation is still structural rather than a property-prediction validation, but it gives a broader test of discriminating power at fixed molecular formula.

Table 3. Distinct-value counts for descriptors on alkane skeleton families C_nH_{2n+2} , $8 \leq n \leq 10$, after rounding numerical values to 10^{-10} .

n	Skeletons	W	R	M_1	LE	$\mathcal{A}$	$\mathcal{B}$
8	18	16	16	6	18	18	18
9	35	16	28	7	35	35	35
10	75	40	49	8	75	75	75

7 Comparison with standard descriptors and preliminary boiling-point test

7.1 Comparison against Wiener, Randić, Zagreb, and Laplacian energy

The new totals $\mathcal{A}$ and $\mathcal{B}$ should be read against established structural descriptors such as the Wiener index W , the Randić connectivity index R , the first Zagreb index M_1 , and the ordinary Laplacian energy LE [8,9,14,16]. On the octane family, the most relevant comparative question is not whether the response descriptors dominate every classical index in every task, but whether they add structurally meaningful discrimination and whether they collapse to information already contained in static descriptors.

Table 4 records how many distinct values each descriptor assumes on the full set of all 18 hydrogen-suppressed octane skeletons after rounding numerical values to 10^{-10} . The first Zagreb index is heavily degenerate because it depends only on the degree multiset. The Wiener and Randić indices perform substantially better, but each still leaves two collisions. By contrast, no collisions are observed for LE, $\mathcal{A}$, and $\mathcal{B}$ under this numerical criterion.

Table 4. Distinct-value count for several standard descriptors on the full octane family after rounding to 10^{-10} .

Descriptor	Distinct values on 18 octanes	Example collision
W	16	O8/O9 and O10/O12
R	16	O3/O7 and O6/O8
M_1	6	degree-sequence classes
LE	18	none
$\mathcal{A}$	18	none
$\mathcal{B}$	18	none

Numerical separation alone does not imply non-redundancy, because LE also separates this family under the same criterion. However, the response descriptors do not merely reproduce the ordering induced by the unperturbed Laplacian energy. For example, for 3-methylheptane (O_3) and

2-methylheptane (O_5) one has

$$\text{LE}(O_3) = 10.4556 > 10.4408 = \text{LE}(O_5),$$

whereas

$$\mathcal{A}(O_3) = 13.7670 < 14.7672 = \mathcal{A}(O_5),$$

$$\mathcal{B}(O_3) = 3.3887 < 3.8661 = \mathcal{B}(O_5).$$

Thus the response descriptors encode a different ranking principle, namely deletion sensitivity rather than only the size-adjusted unperturbed spectrum. In addition, unlike all of the global static descriptors in Table 4, the present framework also supplies the local profiles $v \mapsto \alpha_G(v)$ and $e \mapsto \beta_G(e)$.

The absolute value also has a concrete role in the computations. For the alkane-tree families C_8 , C_9 , and C_{10} considered here, all vertex-deletion signed changes $\ell_G(v)$ are nonnegative, so the atom-response total agrees with the corresponding signed total on these families. Bond deletion is different: the same screen contains negative signed bond changes, namely 17 of 126 edge deletions for C_8 , 25 of 280 for C_9 , and 78 of 675 for C_{10} . Hence the absolute bond-response total $\mathcal{B}$ prevents cancellation already in the present numerical experiments. More generally, the sign of a deletion change is structurally meaningful, but the absolute response records how large the perturbation is irrespective of direction.

7.2 Preliminary boiling-point test on representative octane isomers

A minimal property-oriented check can be carried out on the six representative octane isomers from Section 6 by using standard normal boiling points from the NIST Chemistry WebBook [12]. Table 5 lists the boiling points together with three classical descriptors and the new response totals. The purpose of this test is deliberately limited: it is meant to determine whether the new descriptors follow a chemically sensible trend on a standard alkane family, not to claim a finished QSPR model.

The absolute values differ in scale, so Table 6 summarises the Pearson and Spearman correlations with boiling point. On this six-isomer set the

Table 5. Representative octane isomers: boiling points and selected descriptors.

Isomer	T_{boil} (K)	W	R	M_1	LE	$\mathcal{A}$	$\mathcal{B}$
n-octane	398.7	84	3.9142	26	10.0547	12.9323	2.8304
2-methylheptane	390.7	79	3.7701	28	10.4408	14.7672	3.8661
3-methylheptane	392.0	76	3.8081	28	10.4556	13.7670	3.3887
2,3-dimethylhexane	389.0	70	3.6807	30	11.0583	17.6245	5.4730
2,2-dimethylhexane	380.0	71	3.5607	32	11.0955	18.1184	5.7372
2,2,4-trimethylpentane	372.4	66	3.4165	34	11.2498	19.6956	6.5025

response totals have strong negative Pearson correlations (-0.923 for $\mathcal{A}$ and -0.919 for $\mathcal{B}$) and perfect negative Spearman rank correlation. This behaviour is chemically reasonable: more strongly branched skeletons have larger deletion responses and lower boiling points. At the same time, the classical Randić and first Zagreb indices are at least as strong on this small sample, so the present evidence supports complementarity rather than replacement.

Table 6. Correlation of selected descriptors with normal boiling point on the six-isomer test set.

Descriptor	Pearson r	Spearman ρ
W	0.888	0.886
R	0.991	1.000
M_1	-0.986	-0.986
LE	-0.889	-0.943
$\mathcal{A}$	-0.923	-1.000
$\mathcal{B}$	-0.919	-1.000

Figure 8 visualises the inverse relation between $\mathcal{A}$ and the normal boiling point on the six-isomer set. The especially informative pair is 2-methylheptane versus 3-methylheptane: the boiling points satisfy $390.7\text{ K} < 392.0\text{ K}$, and the response totals follow the same direction, whereas LE orders the pair in the opposite way. This does not establish predictive superiority, but it does show that the response descriptors can supply chemically aligned discrimination not captured by the ordinary Laplacian energy alone.

The comparative evidence therefore supports a moderate claim. The

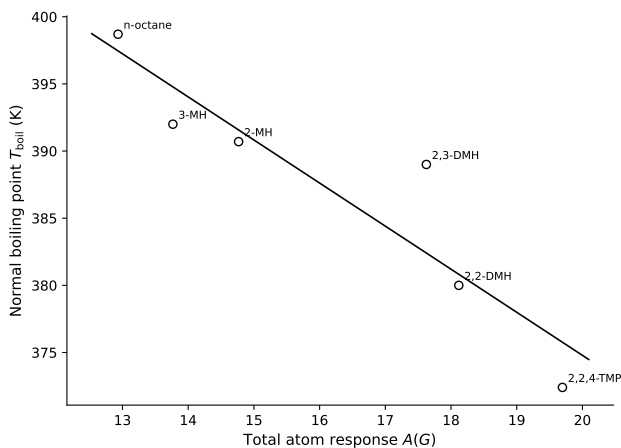


Figure 8. Normal boiling point versus total atom response on the six-isomer octane test set. The trend is chemically sensible but should be interpreted as preliminary only.

descriptors $\mathcal{A}$ and $\mathcal{B}$ are mathematically explicit, locally interpretable, and structurally discriminating. They also show a chemically sensible signal on a small property-oriented benchmark. However, the current data do not justify claiming that they outperform the strongest classical descriptors or that they already constitute a validated QSPR/QSAR tool.

8 Discussion: novelty, chemical relevance, and limitations

The descriptor pair $(\mathcal{A}, \mathcal{B})$ is obtained by combining a standard spectral quantity—Laplacian energy—with vertex- and edge-deletion perturbations. The novelty therefore lies not in inventing an unrelated spectral paradigm, but in introducing a chemically interpretable *absolute-response* reformulation that converts deletion-induced energy changes into local and global sensitivity descriptors. The manuscript now makes this positioning explicit. Lemma 1 and the vertex-deletion comparison are tied directly to Moon and Park [13]; Theorem 1 is presented only as an elementary universal estimate, not as a sharper replacement; and the star family is treated as an illus-

trative benchmark rather than as a new structural theorem. The analytic side of the paper is therefore carried mainly by the response formulation, the transparent atom-response estimate, the bond-response bound that is sharp for every fixed graph order, and exact benchmark computations. The chemical side is carried by the exhaustive alkane-skeleton discrimination, the comparison with standard descriptors, the signed-versus-absolute interpretation, and the preliminary boiling-point check.

The comparative results sharpen the appropriate claim. On the full octane family, $\mathcal{A}$ and $\mathcal{B}$ are as discriminating as ordinary Laplacian energy and more discriminating than the tested Wiener, Randić, and Zagreb indices in terms of numerical collision count after rounding to 10^{-10} . On the small boiling-point test, however, the strongest classical indices remain at least as competitive numerically. The present descriptors should therefore be described as new mathematically explicit descriptors with preliminary chemical discrimination, not as fully validated replacements for established QSPR variables.

The current evidence remains limited from a QSPR/QSAR perspective. Octane isomers are structurally transparent and chemically meaningful as a first benchmark, but they do not support broad predictive claims across heterogeneous molecular classes. Larger homologous series, broader constitutional-isomer families, and external experimental data sets are still required before stronger chemical claims would be justified.

A further reason for keeping both local profiles and global totals is that they serve different interpretive roles. The totals $\mathcal{A}(G)$ and $\mathcal{B}(G)$ are convenient for ranking molecular skeletons, but the profiles retain site-level information and therefore indicate which atom or bond deletions are responsible for the total response. This distinction is important for chemical use: two graphs can have similar global values while concentrating their response at different local environments. Consequently, the proposed descriptors should be used together with their profiles, and not only as single scalar indices, when structural interpretation is required.

The most natural next steps are the following.

- (i) Test larger alkane families and additional constitutional-isomer sets to assess the stability of the discrimination pattern.

- (ii) Compare $(\mathcal{A}, \mathcal{B})$ with established degree-based and spectral descriptors on benchmark QSPR/QSAR data sets.
- (iii) Study weighted variants for heteroatom-containing graphs, bond-order models, or interaction-weighted molecular networks.
- (iv) Investigate extremal problems for molecular trees of fixed order and maximum degree 4 in order to sharpen the mathematical theory.

9 Conclusion

We introduced two perturbative spectral descriptors for molecular graphs: atom-deletion Laplacian response and bond-deletion Laplacian response. The first quantifies how strongly Laplacian energy reacts to deletion of an atom, while the second measures the analogous effect under deletion of a bond. The revised manuscript explicitly separates this absolute-response viewpoint from signed local Laplacian-energy quantities. The central mathematical results are an elementary degree-dependent upper bound for the atom response, a global atom-response estimate, a universal bond-response bound that is sharp for every fixed graph order, and exact benchmark computations for complete graphs and stars. The atom-response bound is not claimed to improve the sharper local estimate of Moon and Park; rather, it supplies a direct trace-norm estimate for the response descriptor.

The octane-family calculations show that $\mathcal{A}$ and $\mathcal{B}$ are structurally discriminating: both totals show no collisions on the 18 hydrogen-suppressed octane skeletons after rounding to 10^{-10} , and the local profiles identify the most deletion-sensitive atoms and bonds. The comparison with standard descriptors also shows that the response totals are not mere reparameterisations of ordinary Laplacian energy, because they can reverse the ordering induced by LE on chemically relevant isomer pairs.

The small six-isomer boiling-point test supports only a measured chemical claim. The new descriptors track the expected branching trend and supply preliminary chemical discrimination, but the data are not strong enough to claim predictive superiority over the best classical indices. The

most important next step is therefore external validation on larger molecular families and experimental-property data sets. Even at the present stage, however, the response-based viewpoint developed here provides a concrete bridge between Laplacian spectral theory and chemically motivated structural discrimination.

Declarations

Data availability

The descriptor computations are reproducible from the algorithm described in Appendix A and from the accompanying CSV files. The preliminary boiling-point values used in Section 7 were taken from the NIST Chemistry WebBook [12]. Distinct-value counts in the numerical tables were computed after rounding descriptor values to 10^{-10} .

Appendix A. Computational protocol and reproducibility

For each molecular graph G , the numerical values in Section 6 were obtained from the Laplacian eigenvalues of G and of the deletion graphs $G - v$ and $G - e$. A concise reproducible workflow is as follows.

- Step 1. Construct the hydrogen-suppressed molecular graph G .
- Step 2. Compute the Laplacian spectrum of G and evaluate $\text{LE}(G)$.
- Step 3. For each vertex $v \in V(G)$, form $G - v$, compute $\text{LE}(G - v)$, and evaluate $\alpha_G(v) = |\text{LE}(G) - \text{LE}(G - v)|$.
- Step 4. For each edge $e \in E(G)$, form $G - e$, compute $\text{LE}(G - e)$, and evaluate $\beta_G(e) = |\text{LE}(G) - \text{LE}(G - e)|$.
- Step 5. Sum the local responses to obtain $\mathcal{A}(G) = \sum_v \alpha_G(v)$ and $\mathcal{B}(G) = \sum_e \beta_G(e)$.

Distinct-value counts reported in the numerical tables were computed after rounding descriptor values to 10^{-10} . For the exhaustive octane-family screen we generated all nonisomorphic trees on 8 vertices with maximum degree at most 4. This graph-theoretic characterisation matches the hydrogen-suppressed skeletons of the constitutional isomers of octane. The labels $O_1, \dots, O_{18}$ used in Section 6 and Appendix B order these graphs by increasing $\mathcal{A}$ (and then by $\mathcal{B}$ when needed to break ties). For the named octane isomers, the skeletons were also hand-constructed from the corresponding IUPAC branching pattern and checked against the nonisomorphic-tree output.

Appendix B. Complete descriptor table for the octane family

Table 7 gives the label, name, and degree sequence of each octane skeleton. Table 8 gives the corresponding numerical descriptors.

Table 7. Labels, names, and degree sequences for the octane family.

Label	Isomer	Degree sequence
O1	n-octane	(2, 2, 2, 2, 2, 2, 1, 1)
O2	3-ethylhexane	(3, 2, 2, 2, 2, 1, 1, 1)
O3	3-methylheptane	(3, 2, 2, 2, 2, 1, 1, 1)
O4	3-ethyl-3-methylpentane	(4, 2, 2, 2, 1, 1, 1, 1)
O5	2-methylheptane	(3, 2, 2, 2, 2, 1, 1, 1)
O6	3,4-dimethylhexane	(3, 3, 2, 2, 1, 1, 1, 1)
O7	4-methylheptane	(3, 2, 2, 2, 2, 1, 1, 1)
O8	3-ethyl-2-methylpentane	(3, 3, 2, 2, 1, 1, 1, 1)
O9	3,3-dimethylhexane	(4, 2, 2, 2, 1, 1, 1, 1)
O10	2,4-dimethylhexane	(3, 3, 2, 2, 1, 1, 1, 1)
O11	2,3-dimethylhexane	(3, 3, 2, 2, 1, 1, 1, 1)
O12	2,2-dimethylhexane	(4, 2, 2, 2, 1, 1, 1, 1)
O13	2,5-dimethylhexane	(3, 3, 2, 2, 1, 1, 1, 1)
O14	2,2,3-trimethylpentane	(4, 3, 2, 1, 1, 1, 1, 1)
O15	2,3,3-trimethylpentane	(4, 3, 2, 1, 1, 1, 1, 1)
O16	2,2,4-trimethylpentane	(4, 3, 2, 1, 1, 1, 1, 1)
O17	2,3,4-trimethylpentane	(3, 3, 3, 1, 1, 1, 1, 1)
O18	2,2,3,3-tetramethylbutane	(4, 4, 1, 1, 1, 1, 1, 1)

Table 8. Laplacian-response descriptor values for the octane family.

Label	LE	$\mathcal{A}$	$\mathcal{B}$	$\max \alpha$	$\max \beta$
O1	10.0547	12.9323	2.8304	2.1540	0.5906
O2	10.3898	13.7436	3.4519	3.2469	0.9257
O3	10.4556	13.7670	3.3887	2.4844	0.9915
O4	10.9443	14.6723	4.0038	4.0871	1.1027
O5	10.4408	14.7672	3.8661	2.1838	1.0122
O6	10.8693	14.7903	4.4281	2.8980	1.2125
O7	10.3702	15.2113	4.0432	2.9416	0.9416
O8	10.7826	15.7306	5.0663	3.6397	1.3539
O9	10.9604	16.7787	5.1426	4.1032	1.5317
O10	10.8418	16.9197	4.8279	3.4132	1.4132
O11	11.0583	17.6245	5.4730	3.6297	1.5861
O12	11.0955	18.1184	5.7372	3.6956	1.2671
O13	11.1272	18.6102	5.7687	2.8415	1.1648
O14	11.5740	19.4026	6.5428	4.1741	1.7456
O15	11.6911	19.6385	6.5189	4.8339	1.7287
O16	11.2498	19.6956	6.5025	4.3926	1.2498
O17	11.6499	20.7121	7.1763	4.2214	1.6876
O18	12.2915	22.5404	8.8204	5.4344	2.2915

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