ACS Guidelines for Presenting Mathematical Information

ABSTRACT: Mathematical expressions are, by nature, often complex, which can make them difficult to present in a way that is clear and concise, as well as aesthetically pleasing. In what follows, we offer some brief guidelines for the presentation of mathematical formulas to indicate how the math in your manuscript will be composed when it is published. Math content is converted to our XML-based composition program from the native files (Word, TeX, etc.) submitted by the authors. Minor inconsistencies in size and alignment of equations and characters sometimes result from the composition program. All composed expressions, however, meet ACS specifications for layout and formatting. More detailed information on style guidelines for math can be found in the ACS Guide to Scholarly Communication online at https://pubs.acs.org/doi/full/10.1021/acsguide.50402.

GENERAL STYLE

ACS employs several mathematical style conventions to maintain consistency and clarity with respect to character style, spacing, numbering, abbreviations, and units of measure. Examples are given in the following:

- Italic type
  - variables: T for temperature
  - axes: x axis
  - planes: ab plane
  - components of vectors and tensors: $a_1 + b_1$
  - elements of determinants and matrices: g_n
  - constants: k_B, the Boltzmann constant
  - functions: $f(x)$
- Roman
  - numerals: 1, 2, 3, ...
  - equation punctuation and enclosing marks: (a, b)
  - most operators: $a + b$
  - units of measure and time: mg, K, mL
  - nonmathematical quantities or symbols: S_1, molecular state; s, atomic orbital
  - multiple-letter abbreviations for variables: IP, ionization potential
  - mathematical constants: e, the base of the natural logarithm, 2.71828...
  - nonvariable subscripts and superscripts: weight-average molecular weight, M_w
- Boldface type
  - vectors: $\mathbf{x} = a + b$
  - tensors: $\boldsymbol{\tau} = [\mathbf{T}_1\mathbf{T}_2\mathbf{T}_3]$
  - matrices: $\mathbf{m} = \begin{bmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{bmatrix}$
  - multidimensional physical quantities: $\mathbf{H}$, magnetic field strength

Greek letters can be used anywhere that a Latin letter is used; lowercase Greek letters are italicized, and uppercase are set in roman type. Spacing is determined by the function of mathematical operators. Operators that function as verbs or conjunctions, that is, have numbers (or a variable and a number) on both sides, have space all around the operators. When they are used as adjectives, with one number that is not part of a mathematical operation, the symbol is closed up to the number (e.g., a conversion of >50%). With the exception of some standard abbreviations that never need to be defined, abbreviations that are used only in the context of mathematical equations should be defined the first time that they are used. Units of measure do not need to be defined. They should be abbreviated when they accompany numbers, with a space between the number and the unit (with exceptions for percent, angular degree, angular minute, and angular second symbols), and left without a period (with an exception: in. for inch). Surnames that are used for units of measure should be lowercase

EQUATIONS

Equations can be presented as in-line or displayed. When an equation is short and will not be referred to again, it can be run into the text either linearized or built up.

For example:

...described by a Hamiltonian $H(\mathbf{r}, \mathbf{p}) = K(\mathbf{p}) + U(\mathbf{r})$ with kinetic energy $K(\mathbf{p})$ and potential energy $U(\mathbf{r})$ which generates forces $F_1(\mathbf{r})$, ..., $F_{dN}(\mathbf{r})$, $F_\alpha(\mathbf{r}) = -\partial U(\mathbf{r})/\partial r_\infty$, and $\alpha = 1, ..., dN$.

...to recognize that $\frac{1}{N}\int \rho(\mathbf{r})\,\mathrm{d}\mathbf{r}$, where...

...should be interpreted as $\frac{1}{\sqrt{2}}(\mathrm{T}_\mathrm{R}^0\mathrm{S}_\mathrm{S}^0 + \mathrm{S}_\mathrm{R}^0\mathrm{T}_\mathrm{S}^0)$ because...

In-text equations are punctuated as parts of the sentences in which they are contained, including closing punctuation.

Display equations are used for numbered equations, long equations, and complicated equations that require more vertical space than is available on a single line of text.

$$m_\alpha {v_\alpha}^2 + \frac{L}{L+2} Q \sum_{k=1}^{L} \mathrm{Q}_1 (v_{1,\alpha}^{(k)})^2 = Lk_\mathrm{B}T \tag{1}$$

$$\mathrm{d}v_{2,\alpha}^{(k)} = \frac{G(v_{1,\alpha}^{(k)})}{\mathrm{Q}_2}\,\mathrm{d}t - \gamma v_{2,\alpha}^{(k)}\,\mathrm{d}t + \sigma\,\mathrm{d}w_\alpha^{(k)} \tag{2}$$

Display equations can be numbered using any consistent system of sequencing with unique numbers for all equations. Number labels are positioned on the lower right-hand side of the equation. End punctuation is not used in display equations. Equations should not contain extraneous text information that is not part of the equation itself. To cite an equation in text, use the abbreviation "eq" if it is not the first word in the sentence. Spell out "equation" when it is the first word of a sentence or when it is not accompanied by a number. The plural of "eq" is "eqs".

Alignment and Indentation. Most equations are broken at their operators. This varies depending on the size, length, and content of specific equations.

$$\begin{aligned} U(\mathbf{r}) &= U_{\mathrm{bond}}(\mathbf{r}) + U_{\mathrm{angle}}(\mathbf{r}) + U_{\mathrm{UB}}(\mathbf{r}) + U_{\mathrm{imp}}(\mathbf{r}) \\ &\quad + U_{\mathrm{tors}}(\mathbf{r}) + U_{\mathrm{vdW}}(\mathbf{r}) + U_{\mathrm{elec}}^{\mathrm{perm}}(\mathbf{r}) + U_{\mathrm{elec}}^{\mathrm{ind}}(\mathbf{r}) \end{aligned} \quad (3)$$

$$\begin{aligned} U_{\mathrm{elec}}^{\mathrm{slow}}(r) &= \tilde{U}_{\mathrm{real}}^{\mathrm{long}}(r) + \tilde{U}_{\mathrm{recip}}(r;\, k_{\mathrm{max}}) \\ &\quad - \sum_i \sum_{j>i} (1 - \delta_{ij}^0) q_i q_j \frac{\mathrm{erf}(\alpha r_{ij}^0)}{r_{ij}^0} S(r_{ij}^0 - r_{\mathrm{elec}}^{\mathrm{res}}) \end{aligned} \quad (4)$$

Breaking Equations. Long equations should typically be broken before an operator. Equations should not be broken after integral, product, and summation signs; after trigonomic and other functions set in roman type; or before derivatives.

$$\begin{aligned} \tilde{U}_{\mathrm{real}}(\mathbf{r};\, r_{\mathrm{real}}) &= \sum_{\mathbf{n}} \sum_{i=1}^{N} \sum_{j \geq i}^{N} (1 - \delta_{ij}^{\mathbf{0}}) q_i q_j \frac{\mathrm{erfc}(\alpha r_{ij}^{\mathbf{n}})}{r_{ij}^{\mathbf{n}}} \\ &\quad [1 - \Theta(r_{ij}^{\mathbf{n}} - r_{\mathrm{real}})] \end{aligned} \quad (5)$$

$$\begin{aligned} \rho_{\mathrm{isok}} &= \mathrm{e}^{-\beta/2 \sum_{\alpha=1}^{\mathrm{d}N} \sum_{k=1}^{L} Q_2 (v_{2,\alpha}^{(k)})^2} \mathrm{e}^{-\beta U(\mathbf{r})} \\ &\quad \prod_{\alpha=1}^{\mathrm{d}N} \delta \left(m_\alpha {v_\alpha}^2 + \frac{L}{L+1} \sum_{k=1}^{L} Q_1 (v_{1,\alpha}^{(k)})^2 - L k_{\mathrm{B}} T \right) \end{aligned} \quad (6)$$

SUBSCRIPTS AND SUPERSCRIPTS

Single subscripts and superscripts are set flush against their accompanying character.

X_1
y_{10}
X^2
10^2
$X^{1/2}$

Subscripts and superscripts can be either staggered or stacked. If the superscript is a power, it should be staggered. Other chemical conventions may require either staggering (e.g., oxidation numbers, ionic charge) or stacking (symmetry operations and structural point groups). Space within subscripts and superscripts should be minimized and used only to avoid misunderstanding.

${X_{\mathrm{b}}}^2$
$y_{\mathrm{d}}^{\mathrm{c}}$
${t_{\mathrm{p}}}^{z-1}$
$x_{\cos x}$

LIMITS (SUMMATION, INTEGRAL, PRODUCT, ETC.)

Limits that are set for in-text expressions are treated as subscripts and superscripts. Please note that in-text expressions compose slightly smaller than their displayed counterparts.

For example:

...where $U_0 = \sum_j {\mu_j}^2/(2\alpha_j)$...

...and then we multiply and divide the first term by $\int_{L_{\mathbf{r}'}} \rho(\mathbf{r}|\mathbf{r}')\, \mathrm{d}\mathbf{r} \approx \sum_{l \in L_{\mathbf{r}'}} \frac{n_{l|k}}{n_k} \equiv N_{L_{\mathbf{r}'}|k}$...

Displayed limits, however, are set as sub-/superscripts or under-/overscripts, except in fractions.

$$\lim_{x \to 0} \qquad \sum_{i=1}^{n} \qquad \prod_{k=2}^{n} \qquad \int_0^1$$

$$E = 1 - \frac{\sum_{i=1}^{n} (O_i - P_i)^2}{\sum_{i=1}^{n} (O_i - \bar{O})^2} \quad (7)$$

The integral symbol will stretch when there are >2 levels in a fraction.

$$\begin{aligned} &\int \frac{x^2 - 29x + 51}{(x-4)^2(x^2+3)}\, \mathrm{d}x \\ &= \int \left(\frac{1}{x-4} - \frac{5}{(x-4)^2} + \frac{-x+2}{(x^2+3)} \right) \mathrm{d}x \end{aligned} \quad (8)$$

$$\int \frac{\frac{3}{x-1} + \frac{1}{2y-y}}{x^2 - x - 6}\, \mathrm{d}x \quad (9)$$

BRACKETING

Bracket size is determined by the information contained within but may vary depending on the specific layout and formatting of individual equations.

$$\begin{aligned} U_{\mathrm{elec}}^{\mathrm{rec}}(\mathbf{r}) &= \frac{2\pi}{L^3} \sum_{\substack{\mathbf{k} \neq (0,0,0) \\ |\mathbf{k}| \leq k_{\mathrm{max}}}} \sum_i \sum_j \Bigg\{ (q_i + \boldsymbol{\mu}_i \cdot \nabla_i + \mathbf{Q}_i :\, \boldsymbol{\Omega}_i) \\ &\quad (q_j + \boldsymbol{\mu}_j \cdot \nabla_j + \mathbf{Q}_j :\, \boldsymbol{\Omega}_j) \mathrm{e}^{2\pi \mathrm{i} \mathbf{k} \cdot (\mathbf{r}_j - \mathbf{r}_i)} \frac{\mathrm{e}^{-k^2/4\alpha^2}}{k^2} \Bigg\} \end{aligned} \quad (10)$$

$$U_{\mathrm{elec}}^{\mathrm{self}} = -\frac{\alpha}{\sqrt{\pi}} \sum_i \left(q_i^2 + \frac{2\alpha^2}{3} |\boldsymbol{\mu}_i|^2 + \frac{4\alpha^4}{5} \|\mathbf{Q}_i\|_F^2 \right) \quad (11)$$

VECTOR, BRA-KET, MATRICES, SETS, ETC.

In what follows, we show additional examples of mathematical expressions. Note that when composed, the spacing and alignment of some expressions are imprecise. In particular, in bra-ket notation, the vertical bar is composed smaller than the angle brackets. Some symbols, such as the set symbols, have a fixed size.

Vector notation

$$\vec{A} = X + Y$$

$$\mathbf{A} = x + y$$

$$\hat{A} = X + Y$$

Bra-ket

$$|\Psi^0\rangle \equiv |\Psi\rangle \qquad |\Psi^x\rangle \equiv \frac{\partial |\Psi\rangle}{\partial \mu_x} \quad (12)$$

$$\langle a| = \left\langle \frac{a}{1} \right| \quad (13)$$

$$|a\rangle = \left|\frac{a}{1}\right\rangle \tag{14}$$

$$\langle a|b\rangle = \left\langle \frac{a}{1}\middle|\frac{b}{1}\right\rangle \tag{15}$$

Matrices

$$\begin{pmatrix} a_{1,1} & a_{1,2} & a_{1,3} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & a_{2,3} & \cdots & a_{2,1} \\ \vdots & \vdots & \vdots & \ddots & a_{2,n} \\ a_{m,1} & a_{m,2} & a_{m,3} & \cdots & a_{m,n} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix} \tag{16}$$

Equation 17 illustrates a right-aligned matrix. Note that we will honor the author's preference with respect to alignment.

$$kA = 2\begin{pmatrix} 2 & 1 \\ -4 & 3 \\ 2 & -2 \end{pmatrix} = \begin{pmatrix} 2(2) & 2(1) \\ 2(-4) & 2(3) \\ 2(2) & 2(-2) \end{pmatrix} = \begin{pmatrix} 4 & 2 \\ -8 & 6 \\ 4 & -4 \end{pmatrix} \tag{17}$$

Sets

$$H_{xy} = \langle \Psi^x | \hat{H} | \Psi^y \rangle \quad \forall\ x, y \in \{0, 1, 2, ..., n_v\} \tag{18}$$

$$\sum_y A_{xy} c_y \approx \sum_{\mathbf{n} \in \xi} \frac{\langle \Psi^x | \mathbf{n} \rangle}{\langle \Psi | \mathbf{n} \rangle} \sum_y \frac{\langle \mathbf{n} | \hat{A} | \Psi^y \rangle}{\langle \mathbf{n} | \Psi \rangle} c_y \tag{19}$$

UNAVAILABLE CHARACTERS

Characters that are not available in our text set include the following:

- Italicized uppercase Greek letters
- Colored fonts
- Some bond symbols (e.g., bonds with dashed lines above or below)
- Lowercase fraktur characters
  e.g., $\mathfrak{a}$, $\mathfrak{b}$, $\mathfrak{c}$
- Uppercase fraktur (with the following exceptions: C, H, I, R, and Z)
  $\mathfrak{C}$, $\mathfrak{H}$, $\mathfrak{I}$, $\mathfrak{R}$, $\mathfrak{Z}$
- Some specialized arrows (e.g., maplet arrows)
  $\mapsto$
- Variations of precedes or succeeds characters such as precedes or approximates
  $\precsim$, $\succsim$
- Less than or approximate/greater than or approximate and not approximate variations
  $\lessapprox$, $\gnapprox$
- Looped script ell
  ℓ
- Hex character (Greek upsilon with hook symbol)
  ϒ
- Hebrew aleph symbol
  $\aleph$
- Surface integral and volume integral
  $\oiint$, $\oiiint$

In the event that a character is unavailable, the editor will format the equation with the available characters or process it as a graphic.

Please note that the font available in the Author Direct Correct (ADC) character picker tool is not the same as the font that is used in our production system. For example, a looped ell character appears in the ADC character picker with the other lower case script characters, but this represents the script ell in our font set, which is not looped. When you insert this character, you will get a script ell from our character set, not a looped ell. Looped ell is not available in the characters that we currently support. We are working to resolve this issue in the future.

PAGE-WIDE EQUATIONS

Page-wide equations include any equation that will compose wider than one column width. These include long fractions, long roots, arrays, matrices, and other equations with complicated formatting.

Note that page-wide equations are used sparingly as they can be difficult to compose, resulting in text that does not flow elegantly or in the insertion of unsightly or awkward spacing. Disrupting composition can affect the way that information in the article is conveyed.

In the following, Latin text is used to display the flow of text only. As seen in the following, the text flows down the column until the page-wide equation and then continues below the equation in the left- and right-hand columns.

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Sed at ante. Mauris eleifend, quam a vulputate dictum, massa quam dapibus leo, eget vulputate orci purus ut lorem. In fringilla mi in ligula. Pellentesque aliquam quam vel dolor. Nunc adipiscing. Sed quam odio, tempus ac, aliquam molestie, varius ac, tellus. Vestibulum ut nulla aliquam risus rutrum interdum. Pellentesque lorem. Curabitur sit amet erat quis risus feugiat viverra. Pellentesque augue justo, sagittis et, lacinia at, venenatis non, arcu. Nunc nec libero. In cursus dictum risus. Etiam tristique nisl a nulla. Ut a orci. Curabitur dolor nunc, egestas at, accumsan at, malesuada nec, magna. Nulla facilisi. Nunc volutpat. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Ut sit amet orci vel mauris blandit vehicula. Nullam quis enim. Integer dignissim viverra velit. Curabitur in odio. In hac habitasse platea dictumst. Ut consequat, tellus eu volutpat varius, justo orci elementum dolor, sed imperdiet nulla tellus ut diam. Vestibulum ipsum ante, malesuada quis, tempus ac, placerat sit amet, elit. Sed eget turpis a pede tempor malesuada. Vivamus quis mi at leo pulvinar hendrerit. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. Pellentesque aliquet lacus vitae pede. Nullam mollis dolor ac nisi. Phasellus sit amet urna. Praesent pellentesque sapien sed lacus. Donec lacinia odio in odio. In sit amet elit. Maecenas gravida interdum urna. Integer pretium, arcu vitae imperdiet facilisis, elit tellus tempor nisi, vel feugiat ante velit sit amet mauris. Vivamus arcu. Integer pharetra magna ac lacus. Aliquam vitae sapien in nibh vehicula auctor. Suspendisse leo mauris, pulvinar sed, tempor et, consequat ac, lacus. Proin velit. Nulla semper lobortis mauris. Duis urna erat, ornare et, imperdiet eu, suscipit sit amet, massa. Nulla nulla nisi, pellentesque at, egestas quis, fringilla eu, diam.

$$\exp(\mathrm{i}L\Delta t) = \exp\left(\mathrm{i}L_{\mathrm{N}}\frac{\Delta t}{2}\right)\exp\left(\mathrm{i}L_{\mathrm{v}}^{\mathrm{slow}}\frac{\Delta t}{2}\right)\left\{\exp\left(\mathrm{i}L_{\mathrm{v}}^{\mathrm{im}}\frac{\delta t}{2}\right)\left[\exp\left(\mathrm{i}L_{\mathrm{v}}^{\mathrm{fast}}\frac{\mathrm{d}t}{2}\right)\exp\left(\mathrm{i}L_{\mathrm{r}}\frac{\mathrm{d}t}{2}\right)\right]^{m}\exp\left(\mathrm{i}L_{\mathrm{v}}^{\mathrm{im}}\frac{\delta t}{2}\right)\right\}^{n} \tag{A.1}$$

Donec semper, sem nec tristique tempus, justo neque commodo nisl, ut gravida sem tellus suscipit nunc. Aliquam erat volutpat. Ut tincidunt pretium elit. Aliquam pulvinar. Nulla cursus. Suspendisse potenti. Etiam condimentum hendrerit felis. Duis iaculis aliquam enim. Donec dignissim augue vitae orci. Curabitur luctus felis a metus. Cum sociis natoque penatibus et magnis dis parturient montes, nascetur ridiculus mus. In varius neque at enim. Suspendisse massa nulla, viverra in, bibendum vitae, tempor quis, lorem. Donec dapibus orci sit amet elit. Maecenas rutrum ultrices lectus. Aliquam suscipit, lacus a iaculis adipiscing, eros orci pellentesque nisl, non pharetra dolor urna nec dolor. Integer cursus dolor vel magna. Integer ultrices feugiat sem. Proin nec nibh. Duis eu dui quis nunc sagittis lobortis. Fusce pharetra, enim ut sodales luctus, lectus arcu rhoncus purus, in fringilla augue elit vel lacus. In hac habitasse platea dictumst. Aliquam erat volutpat. Fusce iaculis elit id tellus. Ut accumsan malesuada turpis. Suspendisse potenti. Vestibulum lacus augue, lobortis mattis, laoreet in, varius at, nisi. Nunc gravida. Phasellus faucibus. In hac habitasse platea dictumst. Integer tempor lacus eget lectus. Praesent fringilla augue fringilla dui.

$$\begin{aligned} A &= \frac{I_{\mathrm{Pt4f}}\left[\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{\mathrm{Pd3d}}(E_{\mathrm{ph}})\right]}{I_{\mathrm{Pd3d}}\left[\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}^{\mathrm{Pt4f}}(E_{\mathrm{ph}})\right]} \\ &= \left(\frac{\rho(r)^{\mathrm{Pt}}}{\rho(r)^{\mathrm{Pd}}}\right)\frac{\left\{2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pt4f}})^3 - \lambda^*(E_{\mathrm{kin}}^{\mathrm{Pt4f}})\exp\left[\frac{-R_{\mathrm{core}}}{\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pt4f}})}\right][R_{\mathrm{core}}{}^2 + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pt4f}})R_{\mathrm{core}} + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pt4f}})^2]\right\}}{\left\{\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})\exp\left[\frac{-R_{\mathrm{core}}}{\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})}\right][R_{\mathrm{core}}{}^2 + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})R_{\mathrm{core}} + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})^2] - \lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})\exp\left[\frac{-R}{\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})}\right][R^2 + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})R + 2\lambda^*(E_{\mathrm{kin}}^{\mathrm{Pd3d}})^2]\right\}} \end{aligned} \tag{A.2}$$

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Sed at ante. Mauris eleifend, quam a vulputate dictum, massa quam dapibus leo, eget vulputate orci purus ut lorem. In fringilla mi in ligula. Pellentesque aliquam quam vel dolor. Nunc adipiscing. Sed quam odio, tempus ac, aliquam molestie, varius ac, tellus. Vestibulum ut nulla aliquam risus rutrum interdum. Pellentesque lorem. Curabitur sit amet erat quis risus feugiat viverra. Pellentesque augue justo, sagittis et, lacinia at, venenatis non, arcu. Nunc nec libero. In cursus dictum risus. Etiam tristique nisl a nulla. Ut a orci. Curabitur dolor nunc, egestas at, accumsan at, malesuada nec, magna. Nulla facilisi. Nunc volutpat. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Ut sit amet orci vel mauris blandit vehicula. Nullam quis enim. Integer dignissim viverra velit. Curabitur in odio. In hac habitasse platea dictumst. Ut consequat, tellus eu volutpat varius, justo orci elementum dolor, sed imperdiet nulla tellus ut diam. Vestibulum ipsum ante, malesuada quis, tempus ac, placerat sit amet, elit.

If you have questions or comments, please contact ACS Support Services at support@services.acs.org.