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¹A.O.(Author One) contributed equally to this work with A.T. (Author Two) (remove if not applicable).

²To whom correspondence should be addressed. E-mail: author.twoemail.com



Fig. 1. Placeholder image of a frog with a long example legend to show justification settina.

Table 1. Comparison of the fitted potential energy surfaces and ab initio benchmark electronic energy calculations

Species	CBS	CV	G3
1. Acetaldehyde	0.0	0.0	0.0
Vinyl alcohol	9.1	9.6	13.5
Hydroxyethylidene	50.8	51.2	54.0

nomenclature for the TSs refers to the numbered species in the table.

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- M Belkin, P Nivogi, Using manifold stucture for partially labeled classification in Advances in neural information processing systems. pp. 929-936 (2002)
- 2. P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. Geom. & Funct. Analysis GAFA 4, 373-398 (1994).
- 3. RR Coifman, et al., Geometric diffusions as a tool for harmonic analysis and structure definition of data: Diffusion maps. Proc. Natl. Acad. Sci. United States Am. 102, 7426-7431 (2005)

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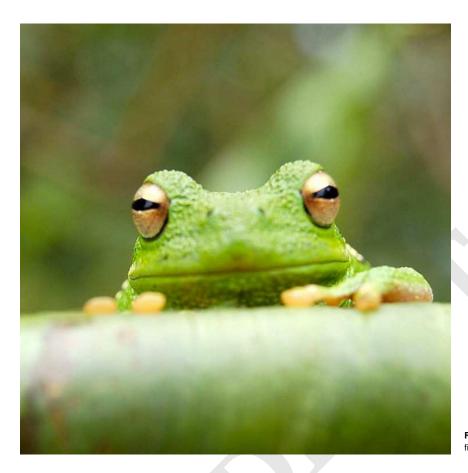


Fig. 2. This legend would be placed at the side of the figure, rather than below it.

$$(x+y)^3 = (x+y)(x+y)^2$$

= $(x+y)(x^2 + 2xy + y^2)$
= $x^3 + 3x^2y + 3xy^3 + x^3$. [1]

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