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

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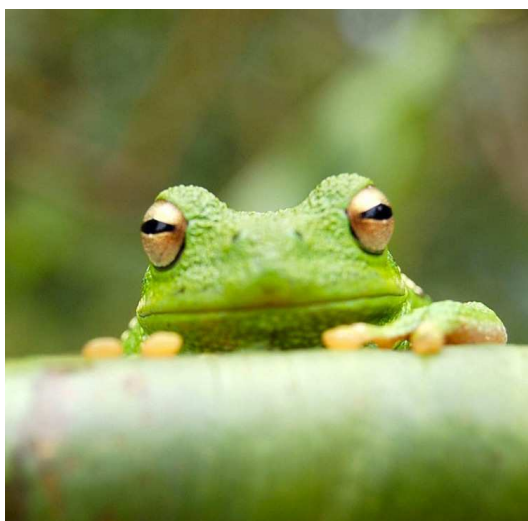


Fig. 1. Placeholder image of a frog with a long example legend to show justification setting.

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
2. Vinyl alcohol	9.1	9.6	13.5
3. Hydroxyethylidene	50.8	51.2	54.0

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

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- 122 1. M Belkin, P Niyogi, Using manifold structure for partially labeled classification in *Advances in neural information processing systems*. pp. 929–936 (2002). 123
- 124 2. P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. *Geom. & Funct. Analysis GAFA* 4, 373–398 (1994). 125
- 126 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). 127



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

$$\begin{aligned}(x + y)^3 &= (x + y)(x + y)^2 \\ &= (x + y)(x^2 + 2xy + y^2) \\ &= x^3 + 3x^2y + 3xy^2 + y^3.\end{aligned}\tag{1}$$