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Fig. 1. Placeholder image of a frog with a long example caption 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
<ol><li>Vinyl alcohol</li></ol>	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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## **Acknowledgments**

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- 1 Belkin M, Niyogi P (2002) Using manifold stucture for partially labeled classification in Advances in neural information processing systems. pp. 929-936
- 2 Bérard P, Besson G, Gallot S (1994) Embedding riemannian manifolds by their heat kernel. Geometric & Functional Analysis GAFA 4(4):373-398.
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 $\label{Fig.2.} \textbf{Fig. 2.} \ \ \textbf{This caption would be placed at the side of the figure, rather than below it.}$ 

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

$$= (x+y)(x^{2} + 2xy + y^{2})$$

$$= x^{3} + 3x^{2}y + 3xy^{3} + x^{3}.$$
[1]