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

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