The GAMESS output file from an attempted geometry optimization of a system containing several hydrogen atoms was used to view the GAMESS output file as a visual model. For each step that was tested, the value listed in the output file as FINAL R-BLYP ENERGY was recorded as the GAMESS total energy for that step. The list of atom coordinates for each step were used in the GAMESS calculations of each of the fragments needed to estimate the total energy using the 2-body and 3-body methods. The nitrogen atom was set as the center of fragment A for each step, while the three oxygen atoms were set as the centers of fragments B, C, and D. These fragments also included whichever hydrogen atoms were closer to the center of that fragment than to the center of any other fragment at that step. Fragments A, B, C, and D are the monomer fragments used in the many-body estimate calculations for the total energy. Since this method uses only 3-body estimates, the nitrogen atom in the monomer fragments that make up that dimer (AR includes all the atoms in A and B). The trimer fragments ABC, ABD, ACD, and BCD are each made up of all the atoms in the monomer fragments that make up that trimer. GAMESS molecular energy calculations were performed on the atoms included in these fourteen fragments at nineteen steps in the reaction. The BLYP**1.18 method and the 6-311G(1-31) basis set were used.

The energy of the 2-body estimate was calculated by summing the terms $V_{ij}$ and $V_{ij} = E_i + E_j + E_{ij}$ is equal to the sum of all the monomer fragment energies and $V_{ij}$ is equal to the sum of six terms accounting for the energy of the interaction between monomers within the dimer fragments. $E_{ij}$ represents the energy of the fragment $i$, $V_{ij} = E_i + E_j + E_{ij}$, and $V_{ij}$ is equal to the sum of six terms accounting for the energy interaction between monomers within the dimer fragments.

$V_{ij} = \left( E_i - E_j \right) + \left( E_i - E_k \right) + \left( E_j - E_k \right) + \left( E_i - E_m \right) + \left( E_j - E_m \right) + \left( E_k - E_m \right)$

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The energy of the 3-body estimate was calculated by summing the terms $V_{ij}$ and $V_{ij} = E_i + E_j + E_{ij}$ is equal to the sum of all the monomer fragment energies and $V_{ij}$ is equal to the sum of six terms accounting for the energy of the interaction between monomers within the dimer fragments. $E_{lij}$ represents the energy of the fragment $i$, $V_{ij} = E_i + E_j + E_{ij}$, and $V_{ij}$ is equal to the sum of six terms accounting for the energy interaction between monomers within the dimer fragments.$V_{ij} = \left( E_i - E_j \right) + \left( E_i - E_k \right) + \left( E_j - E_k \right) + \left( E_i - E_m \right) + \left( E_j - E_m \right) + \left( E_k - E_m \right)$

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