

Ch 121a HW

Patryk Kozlowski

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1. -19.47163529999185 kcal/mol
2. 23.853537629986253 kcal/mol
3. 2.0262830691667495e-05 (1/s)
4. 0.93 Å and 0.95 Å. The latter of the distances is the same as for the highest energy geometry of the scan we performed.
5. 4.671184440000004 kcal/mol
6. A transition state has one imaginary mode because it represents a saddle point of the potential energy surface. It is called imaginary because along this mode the bond is not just vibrating, but is being broken and, thus, the force constant, which measures the strength of a chemical bond, is zero.