



Level of Theory/Basis set	Reaction barrier(+ZPVE) (kcal/mol)
B3LYP/6-31G*	31.3 (30.5)
B3LYP/6-311+G**	34.9 (34.6)
CCSD(T)/aug-ccpVDZ (single point starting from MP2/6-311+G** geometry)	38.4
CCSD(T)/aug-ccpVTZ (single point starting from MP2/6-311+G** geometry)	37.7