Table 1: Zero point energies and imaginary frequencies of the transition state structures calculated for the reactions of guanine with AFB_1 *exo*-8,9-epoxide and DHFF *exo*-4,5-epoxide via different methods.

Method	ZPE^{TS} [kcal/mol] **(a)**	ZPE^{R} [kcal/mol] **(b)**	ω [i cm^{-1}] **(c)**
AFB_1 *exo*-8,9-epoxide			
AM1	265.44	267.69	304
PM3	253.45	255.53	334
HF/6-31G(d)	280.11	281.23	291
HF/6-31+G(d,p)	278.23	279.45	275
HF/6-311++G(d,p)	277.14	278.33	271
B3LYP/6-31G(d)	258.64	259.94	243
B3LYP/6-31+G(d,p)	257.19	258.46	229
B3LYP/6-311++G(d,p)	256.25	257.54	226
DHFF *exo*-4,5-epoxide			
AM1	166.22	167.51	317
PM3	157.09	158.57	150
HF/6-31G(d)	176.98	177.69	285
HF/6-31+G(d,p)	175.98	176.58	268
HF/6-311++G(d,p)	175.25	175.84	265
B3LYP/6-31G(d)	163.03	163.81	260
B3LYP/6-31+G(d,p)	162.24	162.98	230
B3LYP/6-311++G(d,p)	161.66	162.43	228

a) zero point vibrational energy of the transition state

b) zero point vibrational energy of the reactants

c) imaginary frequency value corresponding to the transition state