

Acrolein

Heats of Formation: HF -16.519 kcal/mol
 CI -23.989 kcal/mol

State	Energy	OS	nm

6	5.539155	8.454859	223.860877
13	6.353851	0.823437	195.157239
14	6.910833	1.343430	179.428446
33	9.762560	0.484242	127.015869

Chloro-acrolein

Heats of Formation: HF -25.770 kcal/mol
 CI -30.987 kcal/mol

State	Energy	OS	nm

9	4.768636	0.937833	260.032438
10	5.200222	4.433757	238.451349
12	5.502288	0.148793	225.360807
18	6.413694	0.377669	193.336308

$$\vec{\mu}_{\text{tr}} = - \int \psi_{\text{ex}}^* e \vec{r} \psi_{\text{gs}} d\tau$$

$$f = \left(\frac{8\pi^2}{3} \right) \left(\frac{m\nu}{he^2} \right) |\mu_{\text{tr}}|^2$$