

Molecule	$C_2H_4 \rightarrow C_2F_4$	$NH_3 \rightarrow F_2$
Excitation	${}^3B_2 (\pi \rightarrow \pi^*)$	${}^3A_1 (n \rightarrow \sigma^*)$
Reference	12.63	9.46
HF	13.8764 (30) 31 \rightarrow 1	11.1211 (18) 14 \rightarrow 1
B3LYP	7.0269 (6) 32 \rightarrow 1	2.2178 (1) 14 \rightarrow 1
ω B97	11.2318 (21) 32 \rightarrow 1	6.7329 (8) 14 \rightarrow 1
ω B97X	10.8369 (20) 32 \rightarrow 1	6.1973 (6) 14 \rightarrow 1
ω B97X-D	9.9144 (17) 32 \rightarrow 1	5.0405 (5) 14 \rightarrow 1
LRC- ω PBEh	9.7077 (16) 32 \rightarrow 1	4.8823 (5) 14 \rightarrow 1
M06	7.5926 (6) 32 \rightarrow 1	2.6271 (2) 14 \rightarrow 1
M06-2X	9.3577 (12) 32 \rightarrow 1	5.4936 (6) 14 \rightarrow 1
M06-HF	12.5752 (37) 31 \rightarrow 1	9.3722 (18) 14 \rightarrow 1

Data from Charge-Transfer Examples: Row 1 = Excitation energy (eV);

Row 2 = Excited state; Row 3 = Occ. \rightarrow Virt.