

nitroxy: $1^1A' \rightarrow 2^1A'$

Error in excitation energy (eV)

0.8
0.6
0.4
0.2
0.0

- 6-31+G*
- AVDZ
- AVTZ
- AVQZ

CCSDTQP
CCSDTQ
CCSDT
CC3
CASSCF
CASPT2
PC-NEVPT2
SC-NEVPT2

