

formaldehyde: $1^1A_1 \rightarrow 3^1A_1$

Error in excitation energy (eV)

1.5
1.0
0.5
0.0

CCSDTQP

CCSDTQ

CCSDT

CC3

CASSCF

CASPT2

MS-CASPT2

XMS-CASPT2

PC-NEVPT2

SC-NEVPT2

