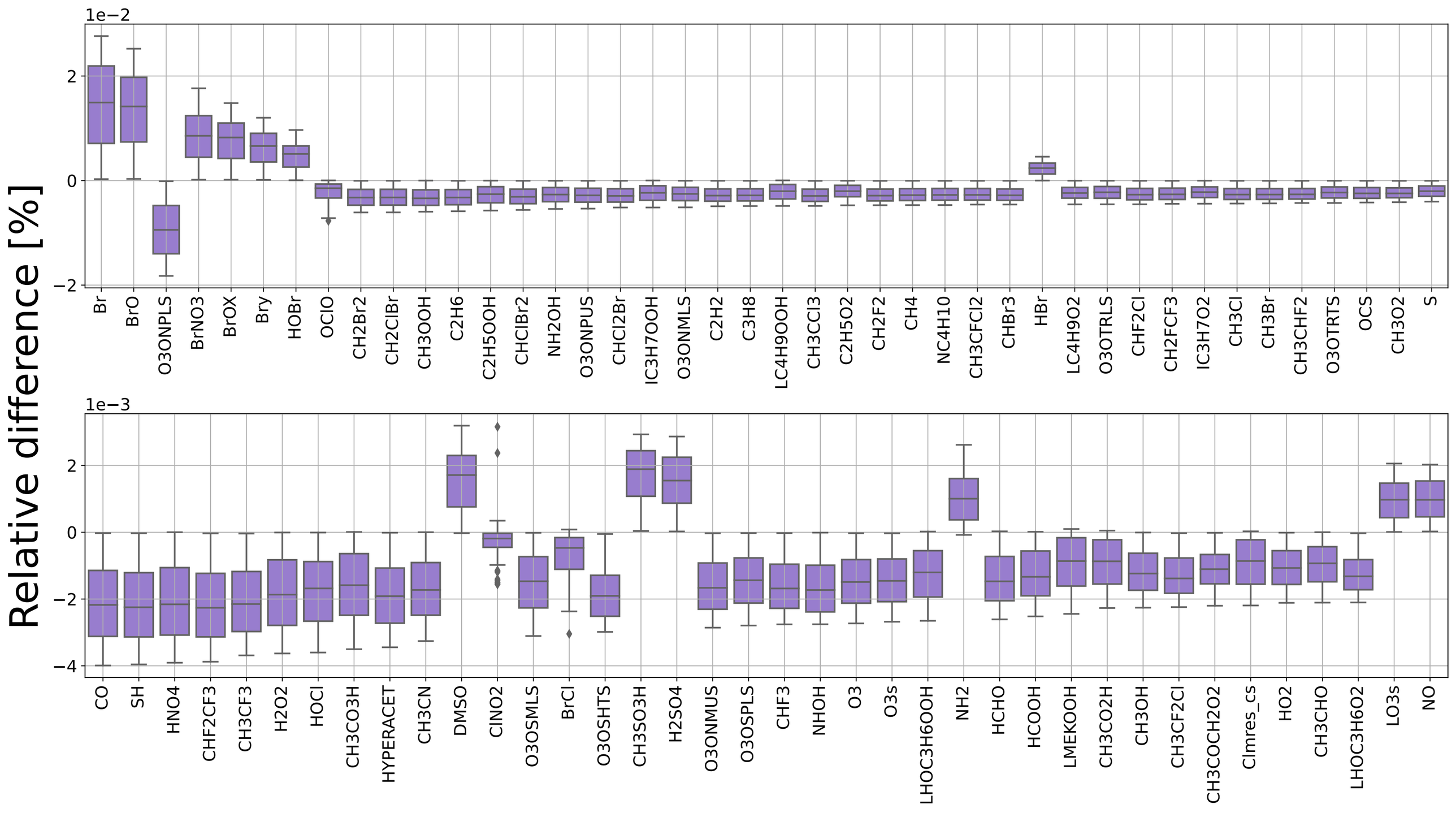

Relative difference [%]
1e−2
2
0
−2
Br
BrO
O3ONPLS
BrNO3
BrOX
Bry
HOBr
OClO
CH2Br2
CH2ClBr
CH3OOH
C2H6
C2H5OOH
CHClBr2
NH2OH
O3ONPUS
CHCl2Br
IC3H7OOH
O3ONMLS
C2H2
C3H8
LC4H9OOH
CH3CCl3
C2H5O2
CH2F2
CH4
NC4H10
CH3CFCl2
CHBr3
HBr
LC4H9O2
O3OTRLS
CHF2Cl
CH2FCF3
IC3H7O2
CH3Cl
CH3Br
CH3CHF2
O3OTRTS
OCS
CH3O2
S
1e−3
2
0
−2
−4
CO
SH
HNO4
CHF2CF3
CH3CF3
H2O2
HOCl
CH3CO3H
HYPERACET
CH3CN
DMSO
ClNO2
O3OSMLS
BrCl
O3OSHTS
CH3SO3H
H2SO4
O3ONMUS
O3OSPLS
CHF3
NHOH
O3
O3s
LHOC3H6OOH
NH2
HCHO
HCOOH
LMEKOOH
CH3CO2H
CH3OH
CH3CF2Cl
CH3COCH2O2
Clmres_cs
HO2
CH3CHO
LHOC3H6O2
LO3s
NO