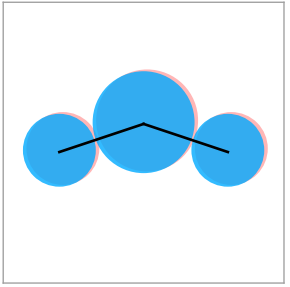
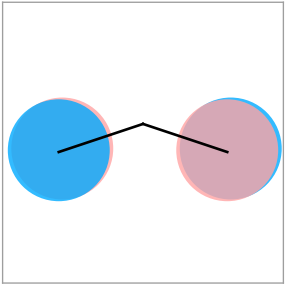
MO 1
2e



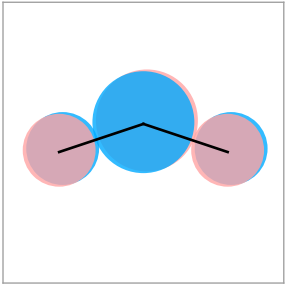
α + 1.41β

MO 2
1e

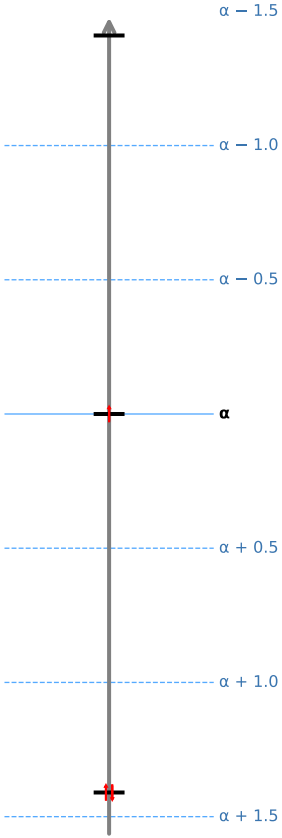


α

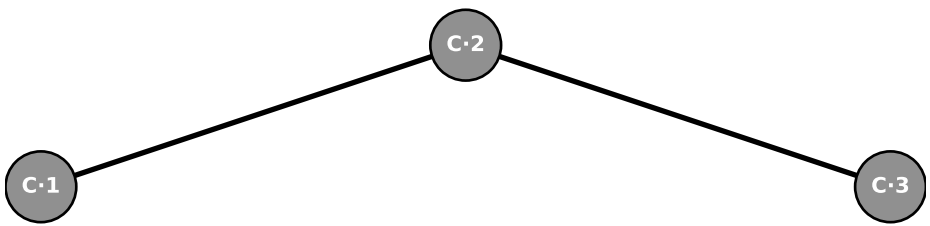
MO 3
0e



α − 1.41β


α − 1.5 β
α − 1.0 β
α − 0.5 β
α
α + 0.5 β
α + 1.0 β
α + 1.5 β
E: 3 α + 2.83 β
E_atom/N: 0.94 |β|
gap: 1.41 |β|
η: 0.71 |β|

σ skeleton




Bond orders and atomic charges