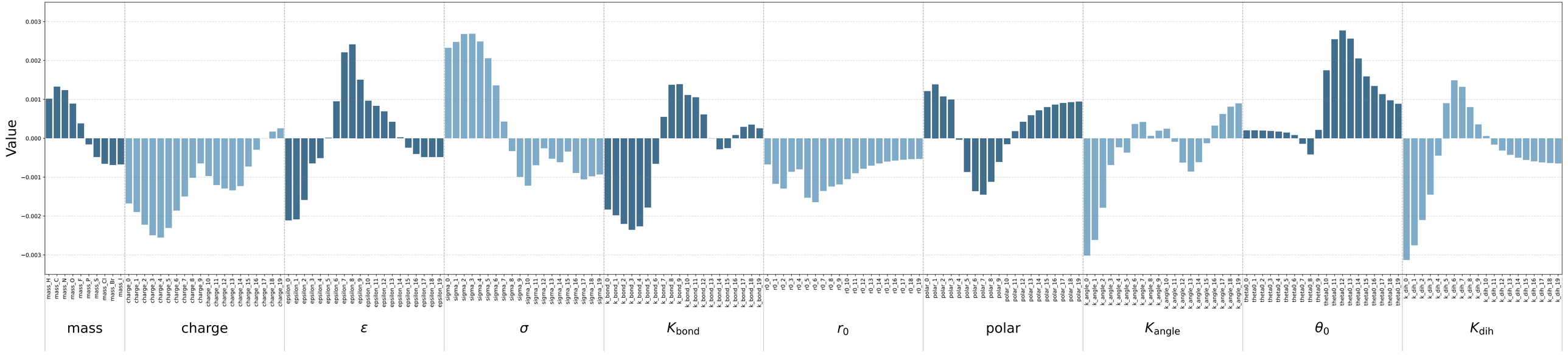
Value
0.003
0.002
0.001
0.000
−0.001
−0.002
−0.003
mass_H
mass_C
mass_N
mass_O
mass_F
mass_P
mass_S
mass_Cl
mass_Br
mass_I
charge_0
charge_1
charge_2
charge_3
charge_4
charge_5
charge_6
charge_7
charge_8
charge_9
charge_10
charge_11
charge_12
charge_13
charge_14
charge_15
charge_16
charge_17
charge_18
charge_19
epsilon_0
epsilon_1
epsilon_2
epsilon_3
epsilon_4
epsilon_5
epsilon_6
epsilon_7
epsilon_8
epsilon_9
epsilon_10
epsilon_11
epsilon_12
epsilon_13
epsilon_14
epsilon_15
epsilon_16
epsilon_17
epsilon_18
epsilon_19
sigma_0
sigma_1
sigma_2
sigma_3
sigma_4
sigma_5
sigma_6
sigma_7
sigma_8
sigma_9
sigma_10
sigma_11
sigma_12
sigma_13
sigma_14
sigma_15
sigma_16
sigma_17
sigma_18
sigma_19
k_bond_0
k_bond_1
k_bond_2
k_bond_3
k_bond_4
k_bond_5
k_bond_6
k_bond_7
k_bond_8
k_bond_9
k_bond_10
k_bond_11
k_bond_12
k_bond_13
k_bond_14
k_bond_15
k_bond_16
k_bond_17
k_bond_18
k_bond_19
r0_0
r0_1
r0_2
r0_3
r0_4
r0_5
r0_6
r0_7
r0_8
r0_9
r0_10
r0_11
r0_12
r0_13
r0_14
r0_15
r0_16
r0_17
r0_18
r0_19
polar_0
polar_1
polar_2
polar_3
polar_4
polar_5
polar_6
polar_7
polar_8
polar_9
polar_10
polar_11
polar_12
polar_13
polar_14
polar_15
polar_16
polar_17
polar_18
polar_19
k_angle_0
k_angle_1
k_angle_2
k_angle_3
k_angle_4
k_angle_5
k_angle_6
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k_angle_8
k_angle_9
k_angle_10
k_angle_11
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k_angle_14
k_angle_15
k_angle_16
k_angle_17
k_angle_18
k_angle_19
theta0_0
theta0_1
theta0_2
theta0_3
theta0_4
theta0_5
theta0_6
theta0_7
theta0_8
theta0_9
theta0_10
theta0_11
theta0_12
theta0_13
theta0_14
theta0_15
theta0_16
theta0_17
theta0_18
theta0_19
k_dih_0
k_dih_1
k_dih_2
k_dih_3
k_dih_4
k_dih_5
k_dih_6
k_dih_7
k_dih_8
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k_dih_10
k_dih_11
k_dih_12
k_dih_13
k_dih_14
k_dih_15
k_dih_16
k_dih_17
k_dih_18
k_dih_19
mass
charge
ε
σ
K_{bond}
r_0
polar
K_{angle}
θ_0
K_{dih}