

Atom type	Adjustment in	Adjustment in
C	$+0.004 \pm 0.003$	$+0.012 \pm 0.003$
O/N	-0.113 ± 0.014	-0.116 ± 0.013
S	-0.017 ± 0.022	-0.018 ± 0.021
O ⁻	-0.166 ± 0.038	-0.175 ± 0.036
N ⁺	-0.169 ± 0.031	-0.186 ± 0.022