Supporting Information

Table 1s. Electronic parameters from the POP multipole refinement for $KMnO_4$ (**1**). p1, p2 and p3 are the population values for the first, second and third monopole functions, respectively. d, q, o, h indicate dipole, quadrupole, octopole and hexadecapole parameters, respectively. The α's for K, Mn and O atoms were fixed to the standard molecular values. The reference Cartesian coordinate system consists of the a, b and c axes.

Atom	p1	p2	p3	d1	d2	d3	q1	q2	q3	q4	q5
K	10.1653	-	8.40(6)	0.00(3)	-	0.05(3)	-0.009(9)	-	0.02(2)	-	-0.01(1)
Mn	10.16(1)	6.9(2)	8.8(3)	-0.02(2)	-	-0.05(2)	-0.016(6)	-	-0.01(1)	-	-0.02(1)
O(1)	1.93(2)	-	6.52(4)	0.09(2)	-	-0.02(2)	-0.002(4)	-	0.001(7)	-	0.001(6)
O(2)	1.93(2)	-	6.54(4)	-0.10(2)	-	-0.01(2)	-0.000(4)	-	-0.009(8)	-	0.014(8)
O(3)	1.93(2)	-	6.51(4)	0.03(1)	0.01(1)	-0.06(1)	-0.002(2)	-0.002(5)	-0.003(4)	-0.008(5)	-0.010(4)

Atom	o1	o2	o3	o4	o5	o6	o7
K	-0.002(3)	-	0.007(8)	-	0.001(2)	-	0.001(2)
Mn	0.000(2)	-	-0.022(4)	-	-0.002(1)	-	-0.001(1)
O(1)	-0.0004(7)	-	0.003(2)	-	-0.0001(5)	-	0.0000(4)
O(2)	-0.0025(7)	-	-0.006(2)	-	-0.0003(5)	-	0.0000(4)
O(3)	-0.0004(4)	0.0002(4)	0.0006(9)	0.003(2)	0.0002(3)	-0.0006(3)	0.0000(2)

Atom	h1	h2	h3	h4	h5	h6	h7	h8	h9
Mn	0.000(1)	-	-	-	0.0004(5)	-	0.0010(7)	-	-0.0013(5)

Table 2s. Electronic parameters from the POP multipole refinement for $KClO_4$ (**2**). p1, p2 and p3 are the population values for the first, second and third monopole functions, respectively. d, q and o indicate dipole, quadrupole and octopole parameters, respectively. The α's for K, Cl and O atoms were fixed to the standard molecular values. The reference Cartesian coordinate system consists of the a, b and c axes.

Atom	p1	p2	p3	d1	d2	d3	q1	q2	q3	q4	q5
K	10.02896	-	7.93(4)	0.05(2)	-	0.03(2)	0.013(7)	-	0.008(9)	-	-0.04(1)
Cl	10.02896	-	5.96(6)	0.01(1)	-	0.01(1)	0.003(3)	-	-0.004(4)	-	-0.008(4)
O(1)	1.94(1)	-	6.32(3)	0.06(1)	-	-0.01(1)	-0.004(3)	-	-0.018(5)	-	0.002(4)
O(2)	1.94(1)	-	6.35(3)	-0.02(1)	-	-0.01(2)	-0.006(3)	-	-0.001(5)	-	-0.002(5)
O(3)	1.94(1)	-	6.30(2)	-0.006(9)	0.00(1)	-0.04(1)	0.007(2)	-0.003(3)	0.005(3)	0.010(4)	-0.002(3)

Atom	o1	o2	o3	o4	o5	o6	o7
K	-0.001(2)	-	0.011(5)	-	-0.003(1)	-	-0.000(1)
Cl	0.0010(5)	-	-0.025(1)	-	-0.0019(3)	-	-0.0004(3)
O(1)	0.0003(4)	-	-0.000(1)	-	0.0010(3)	-	-0.0005(2)
O(2)	-0.0004(4)	-	0.000(1)	-	-0.0009(4)	-	-0.0012(3)
O(3)	0.0003(3)	-0.0005(3)	0.0026(7)	0.001(1)	0.0002(2)	0.0008(2)	0.0006(2)