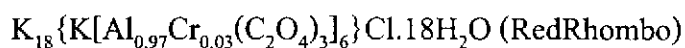


## Appendix

Table 17 Non-Hydrogen Atom Coordinate and Site Occupation Parameters of



| Atom  | x/a        | y/b        | z/c       | PP        |
|-------|------------|------------|-----------|-----------|
| K(1)  | 2/3        | 1/3        | 5/6       |           |
| Al(1) | 0.62537(5) | 0.49921(5) | 0.9086(1) | 0.9710(-) |
| Cr(1) | 0.62537(5) | 0.49921(5) | 0.9086(1) | 0.0290(-) |
| C(1)  | 0.6829(2)  | 0.5998(2)  | 1.0171(4) |           |
| C(2)  | 0.7108(2)  | 0.5674(2)  | 1.0650(4) |           |
| O(1)  | 0.6427(1)  | 0.5722(1)  | 0.9355(3) |           |
| O(2)  | 0.6893(1)  | 0.5198(1)  | 1.0138(3) |           |
| O(11) | 0.6979(1)  | 0.6458(1)  | 1.0583(3) |           |
| O(12) | 0.7481(1)  | 0.5872(1)  | 1.1474(3) |           |
| C(3)  | 0.6583(2)  | 0.4791(2)  | 0.6709(4) |           |
| C(4)  | 0.6364(2)  | 0.4262(2)  | 0.7558(4) |           |
| O(3)  | 0.6595(1)  | 0.5185(1)  | 0.7365(3) |           |
| O(4)  | 0.6190(1)  | 0.4300(1)  | 0.8728(3) |           |
| O(13) | 0.6720(1)  | 0.4799(1)  | 0.5530(3) |           |
| O(14) | 0.6374(1)  | 0.3866(1)  | 0.7075(3) |           |
| C(5)  | 0.5159(2)  | 0.4564(2)  | 0.9060(4) |           |
| C(6)  | 0.5318(2)  | 0.4544(2)  | 1.0548(4) |           |
| O(5)  | 0.5574(1)  | 0.4800(1)  | 0.8274(3) |           |
| O(6)  | 0.5835(1)  | 0.4727(1)  | 1.0692(3) |           |

Table 17 Non-Hydrogen Atom Coordinate and Site Occupation Parameters of

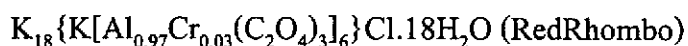
$$\text{K}_{18}\{\text{K}[\text{Al}_{0.97}\text{Cr}_{0.03}(\text{C}_2\text{O}_4)_3]_6\}\text{Cl}\cdot 18\text{H}_2\text{O} \text{ (RedRhombo) (continued)}$$

| Atom  | x/a        | y/b        | z/c       | PP |
|-------|------------|------------|-----------|----|
| O(15) | 0.4683(1)  | 0.4377(1)  | 0.8719(3) |    |
| O(16) | 0.4984(1)  | 0.4385(1)  | 1.1453(3) |    |
| K(2)  | 0.68609(4) | 0.62222(4) | 0.6131(1) |    |
| K(3)  | 0.81552(5) | 0.71117(5) | 1.0083(1) |    |
| K(4)  | 0.63730(4) | 0.40636(4) | 1.1438(1) |    |
| Cl(1) | 2/3        | 1/3        | 4/3       |    |
| O(7)  | 0.6672(1)  | 0.5529(1)  | 1.3758(4) |    |
| O(8)  | 0.7369(2)  | 0.4850(1)  | 1.2781(3) |    |
| O(9)  | 0.5737(2)  | 0.5494(2)  | 0.6117(4) |    |

Table 18 Hydrogen Atom Coordinates and Isotropic Displacement Parameters of  
 $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$  (RedRhomb)

| Atom | x/a       | y/b       | z/c       | U(eq) A**2 |
|------|-----------|-----------|-----------|------------|
| H(1) | 0.6732(-) | 0.5304(-) | 1.4409(-) | * 0.081(-) |
| H(2) | 0.6996(-) | 0.5791(-) | 1.3293(-) | * 0.081(-) |
| H(3) | 0.7554(-) | 0.4774(-) | 1.2147(-) | * 0.075(-) |
| H(4) | 0.7411(-) | 0.5120(-) | 1.2171(-) | * 0.078(-) |
| H(5) | 0.5678(-) | 0.5283(-) | 0.6843(-) | * 0.095(-) |
| H(6) | 0.5861(-) | 0.5798(-) | 0.6551(-) | * 0.095(-) |

Table 19 Non-Hydrogen Atomic Displacement Parameters of



| Atom  | U11       | U22       | U33       | U12       | U13       | U23       |
|-------|-----------|-----------|-----------|-----------|-----------|-----------|
| K(1)  | 2U12      | 2U12      | 0.092(3)  | 0.0405(9) | 0         | 0         |
| Al(1) | 0.0225(7) | 0.0186(6) | 0.0202(7) | 0.0113(6) | 0.0006(5) | 0.0004(5) |
| Cr(1) | 0.0225(7) | 0.0186(6) | 0.0202(7) | 0.0113(6) | 0.0006(5) | 0.0004(5) |
| C(1)  | 0.029(3)  | 0.030(3)  | 0.028(3)  | 0.016(2)  | 0.002(2)  | -0.002(2) |
| C(2)  | 0.027(3)  | 0.031(3)  | 0.026(3)  | 0.016(2)  | 0.003(2)  | 0.001(2)  |
| O(1)  | 0.027(2)  | 0.022(2)  | 0.032(2)  | 0.014(1)  | -0.006(1) | -0.003(1) |
| O(2)  | 0.027(2)  | 0.026(2)  | 0.029(2)  | 0.016(1)  | -0.003(1) | -0.001(1) |
| O(11) | 0.044(2)  | 0.029(2)  | 0.058(2)  | 0.022(2)  | -0.016(2) | -0.018(2) |
| O(12) | 0.042(2)  | 0.046(2)  | 0.048(2)  | 0.027(2)  | -0.024(2) | -0.015(2) |
| C(3)  | 0.018(2)  | 0.024(2)  | 0.027(2)  | 0.009(2)  | -0.001(2) | 0.003(2)  |
| C(4)  | 0.017(2)  | 0.022(2)  | 0.026(2)  | 0.008(2)  | -0.003(2) | 0.001(2)  |
| O(3)  | 0.035(2)  | 0.018(2)  | 0.023(2)  | 0.014(1)  | 0.006(1)  | 0.003(1)  |
| O(4)  | 0.030(2)  | 0.020(2)  | 0.022(2)  | 0.013(1)  | 0.004(1)  | 0.003(1)  |
| O(13) | 0.040(2)  | 0.034(2)  | 0.021(2)  | 0.019(2)  | 0.008(1)  | 0.004(1)  |
| O(14) | 0.032(2)  | 0.022(2)  | 0.031(2)  | 0.016(1)  | -0.004(1) | 0.004(1)  |
| C(5)  | 0.027(2)  | 0.017(2)  | 0.033(3)  | 0.012(2)  | -0.002(2) | -0.000(2) |
| C(6)  | 0.029(3)  | 0.016(2)  | 0.030(3)  | 0.012(2)  | 0.001(2)  | -0.002(2) |
| O(5)  | 0.025(2)  | 0.027(2)  | 0.024(2)  | 0.012(1)  | -0.001(1) | 0.002(1)  |
| O(6)  | 0.025(2)  | 0.029(2)  | 0.023(2)  | 0.013(1)  | 0.000(1)  | 0.001(1)  |
| O(15) | 0.024(2)  | 0.037(2)  | 0.048(2)  | 0.014(2)  | -0.003(2) | 0.005(2)  |
| O(16) | 0.032(2)  | 0.032(2)  | 0.034(2)  | 0.013(2)  | 0.012(2)  | 0.003(2)  |

Table 19 Non-Hydrogen Atomic Displacement Parameters of

$$\text{K}_{18}\{\text{K}[\text{Al}_{0.97}\text{Cr}_{0.03}(\text{C}_2\text{O}_4)_3]_6\}\cdot\text{Cl}\cdot 18\text{H}_2\text{O}$$
 (RedRhombo) (continued)

| Atom  | U11       | U22       | U33       | U12       | U13        | U23        |
|-------|-----------|-----------|-----------|-----------|------------|------------|
| K(2)  | 0.0335(6) | 0.0275(6) | 0.0539(7) | 0.0156(5) | -0.0022(5) | -0.0023(5) |
| K(3)  | 0.0486(8) | 0.0740(9) | 0.0549(8) | 0.0350(7) | -0.0008(6) | -0.0245(7) |
| K(4)  | 0.0308(6) | 0.0387(6) | 0.0292(6) | 0.0160(5) | -0.0014(4) | 0.0046(5)  |
| Cl(1) | 2U12      | 2U12      | 0.028(1)  | 0.0175(5) | 0          | 0          |
| O(7)  | 0.053(2)  | 0.059(3)  | 0.053(2)  | 0.027(2)  | -0.007(2)  | 0.011(2)   |
| O(8)  | 0.067(3)  | 0.071(3)  | 0.039(2)  | 0.048(2)  | 0.007(2)   | 0.006(2)   |
| O(9)  | 0.059(3)  | 0.073(3)  | 0.069(3)  | 0.035(2)  | 0.001(2)   | 0.032(2)   |