Appendix

Table 17 Non-Hydrogen Atom Coordinate and Site Occupation Parameters of $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$ (RedRhombo)

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 $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$ (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 $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$ (RedRhombo)

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 $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$ (RedRhombo)

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 $K_{18}\{K[Al_{0.97}Cr_{0.03}(C_2O_4)_3]_6\}Cl.18H_2O$ (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)