Crystallographic information

Crystal data

Formula	$H_3KMn_2Mo_2O_{10}$
Formula weight	503.87
Crystal system	monoclinic
Space-group	C2/m
a, b, c Å	9.7233(13), 6.6838(10), 7.8774(10)
α, β, γ	90, 116.220(11), 90°
V	459.3(1) $Å^3$
Z	2
d_{calc}	3.643 g cm^{-3}
μ	58.4 cm^{-1}
F_{000}	472

Data collection

Crystal dimensions	0 05 x 0.07 x 0.11 mm
Diffractometer	Enraf-Nonius CAD-4
Radiation, wavelength	Mo Kα, 0.71073 Å
Monochromator	graphite
Temperature	22 °C
$2\theta_{max}$	60°
Index range h, k, l	0→13, 0→9, -10→9

Scan mode	ω-2θ
Scan speed (on ω)	4.1° min^{-1}
Scan width	(1.10 + 0.35tanθ)°
Reference reflections	3, every 3600 s exposure
No. indep. rflns scanned	758 (incl. 45 syst. absences)
R_{int} (on F^2 for 0,k,±1)	0.011

Refinement

Absorption correction	none
Sec. extinction parameter (g)	1.2(10) x 10^{-7}
No. rflns in refinement (N)	651 [$I>1.5\sigma(I)$]
No. parameters (V)	45
Function minimized	$\Sigma w(\|F_o\|-\|F_c\|)^2$
Weighting factor w	$1/\sigma^2(F)$
R(F), wR(F)	0.025, 0.034
S	1.60
Max. Δ/σ, last cycle	0.02
Max., min. in final diff. map	0.75, -0.98 e $Å^{-3}$

$$R(F) = \Sigma||F_o|-|F_c||/\Sigma|F_o| \qquad wR(F) = [\Sigma w(|F_o|-|F_c|)^2/\Sigma w|F_o|^2]^{1/2}$$

$$S = [\Sigma w(|F_o|-|F_c|)^2/(N-V)]^{1/2} \qquad I_o(corr) = I_o(1+2gI_c)$$

Anisotropic thermal parameters (Å^2)

The temperature factor is given by: $T = \exp[-2\pi^2\Sigma_i\Sigma_j U_{ij}h_ih_ja^*_ia^*_j]$

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mo	0.0079(2)	0.0110(2)	0.0102(2)	0.0000	0.00352(17)	0.0000
Mn	0.0154(4)	0.0141(4)	0.0174(4)	-0.0016(3)	0.0058(3)	0.0001(3)
K	0.0182(8)	0.0190(8)	0.0174(8)	0.0000	0.0085(7)	0.0000
01	0.0162(20)	0.0322(25)	0.0164(21)	0.0000	0.0038(17)	0.0000
02	0.0143(13)	0.0147(13)	0.0183(13)	0.0028(11)	0.0049(11)	-0.0031(12)
03	0.0176(20)	0.0171(20)	0.021(2)	0.0000	0.0137(18)	0.0000
04	0.0152(19)	0.0146(19)	0.0186(20)	0.0000	0.0102(16)	0.0000

Contact distances under 3.6 Å

atom	atom	distance	code	atom	atom	distance	code
Mo	03	3.251(4)	5553	01	02	3.438(5)	5563
K	02	2.717(3)	5551	01	02	3.438(5)	5564
K	02	2.717(3)	5652	01	01	3.446(2)	5567
K	02	2.717(3)	5663	01	01	3.446(2)	5467
K	02	2.717(3)	5564	02	04	2.992(4)	4555
K	01	2.826(5)	4555	02	03	3.071(5)	5553
K	01	2.826(5)	5567	02	04	3.125(5)	5553
K	03	3.096(4)	4555	02	03	3.140(4)	4555
K	03	3.096(4)	5567	03	03	3.329(9)	5553
01	H1	1.929	5561	03	04	3.3705(8)	5457
01	04	2.770(6)	5561	04	H2	1.859	6553
01	02	3.383(5)	5567	04	04	2.618(8)	6553
01	02	3.383(5)	5468				

The digits in the code pqrs denote that the second atom is derived from the corresponding atom in the table of atomic coordinates by the action of the symmetry operator numbered s (see below) followed by (p-5), (q-5), and (r-5) unit translations in the +a, +b, and +c directions respectively. For instance, the code 5468 denotes that the second atom has been shifted from x, y, z to (1/2)-x, (-1/2)+y, 1-z.

(1) +x, +y, +z
(2) +x, -y, +z
(3) -x, -y, -z
(4) -x, +y, _z
(5) (1/2)+x, (1/2)+y, +z
(6) (1/2)+x, (1/2)-y, +z
(7) (1/2)-x, (1/2)-y, -z
(8) (1/2)-x, (1/2)+y, -z