Summary

Collection Code 202727

Struct.formula	Mn6 O12 (H2 O)3	Author	Post, J.E.; Bish, D.L.
Space Group	P 1 2/m 1(10)		
Unit Cell	9.789(6) 2.834(1) 9.551(4) 90. 93.72(3) 90.	Title of Article	Rietveld refinement of the todorokite structure
Cell Volume	264.41 A^3 Formula Units per Cell 1		
Temperature	room temperature Pressure atmospheric	Reference	American Mineralogist (1988) 73, p861-p869
PDF-numbers	01-084-1714 38-475 R-value 0.124	Warnings & Comments	1 Warnings / 2 Comments
Remark	High Quality Data		

Details

- Visualization
- Chemistry
- Published Crystal Structure Data
- Standardized Crystal Structure Data

Cell Parameters	9.5510 2.8340 9.7890 90.000 93.720 90.000			
Volume	264.41	Formula Units per Cell	1	Calc. Dens. 3.62
Space Group	P 1 2/m 1(10)	Pearson Symbol	mP27	
Crystal System	monoclinic	Crystal Class	2/m	Laue Class 2/m
Wyckoff Sequence	n4 m4 h a			
Axis Ratios	a/b 3.3701	b/c 0.2895	c/a 1.0249	

Transformation Method	Tidy
Transformation Info	TRANS c,-b,a origin 0 1/2 1/2

Remark

EL	Lbl	OxState	WyckSymb	X	Y	Z	B	SOF
Mn	1	+4.00	1a	0.0000	0.0000	0.0000	0.8000	
Mn	2	+4.00	2n	0.0020	0.5000	0.2640	0.8000	
Mn	3	+4.00	1h	0.5000	0.5000	0.5000	0.8000	
Mn	4	+4.00	2m	0.2410	0.0000	0.5100	0.8000	
O	1	-2.00	2m	0.1160	0.0000	0.6800	1.0000	
O	2	-2.00	2n	0.0690	0.5000	0.9030	1.0000	
O	3	-2.00	2m	0.1100	0.0000	0.1630	1.0000	
O	4	-2.00	2n	0.1500	0.5000	0.4080	1.0000	
O	5	-2.00	2m	0.4120	0.0000	0.4030	1.0000	
O	6	-2.00	2n	0.3340	0.5000	0.6110	1.0000	

Distances & Angles

Select Pairs of Elements

Atom A	Atom B	Atom C
H Mn O	H Mn O	H Mn O

Select from Atom Positions

Configure Bonds & Angles Calculation

- [x] Distance [Å] min: 0.7 max: 3.0
- [ ] Ionic radii [%] min: 80.0 max: 120.0

- Bibliography
- Experimental Information
- Warnings & Comments

Warnings

The coordinates given in the paper contain an error. The values in the database have been corrected.

Comments

For H2 O positions cf. 202725

X(O5) was misprinted as .993, z(O5) as .472

Compare Published & Standardized Structure