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Synthesis and crystal structure of a mixed alkaline-earth powellite, $Ca_{0.84}Sr_{0.16}MoO_4$

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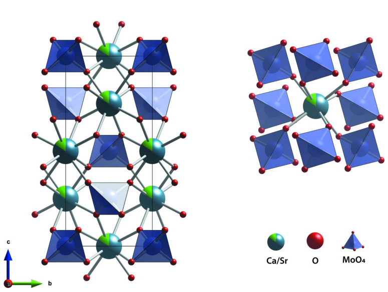
A mixed alkaline-earth powellite, $Ca_{0.84}Sr_{0.16}MoO_4$ (calcium strontium molybdate), was synthesized by a flux method and its crystal structure was solved using single-crystal X-ray diffraction (SC-XRD) data. The compound crystallized in the $I4_1/a$ space group as with a typical $CaMoO_4$ powellite, but with larger unit-cell parameters and unit-cell volume as a result of the partial incorporation of larger Sr cations into the Ca sites within the crystal. The unit cell and volume were well fitted with the trendline calculated from literature values, and the powder X-ray diffraction (P-XRD) pattern of the ground crystal is in good agreement with the calculated pattern from the solved structure.



1. Chemical context

Powellite ($CaMoO_4$) is a naturally occurring mineral with the scheelite ($CaWO_4$) structure and has been studied for different applications including laser materials, phosphors, catalysts, electrodes, and radionuclide waste forms (Kato *et al.*, 2005; Lei & Yan, 2008; Rabuffetti *et al.*, 2014; Peterson *et al.*, 2018; Ryu *et al.*, 2007). Powellites doped with rare-earth elements have broad absorption bands and fluorescence emissions in the visible to near-infrared range (Kim & Kang, 2007; Lei & Yan, 2008; Schmidt *et al.*, 2013), and isostructural $BaMoO_4$ and $SrMoO_4$ crystals have high photoluminescence emission in the visible spectral region (Bi *et al.*, 2008; Lei *et al.*, 2010). Powellite has been investigated for use in a potential electrode with Li cyclability for battery applications (Reddy *et al.*, 2013). Alkaline-earth powellites crystallize during the development of the ceramic-waste forms for radionuclides in the high-level waste (HLW) raffinate stream from aqueous reprocessing of used nuclear fuel (Crum *et al.*, 2019; Peterson *et al.*, 2018).

Various methods have been used to synthesize scheelite-structured crystals including vapor diffusion sol-gel (VDSG), hydrothermal, molten salt reaction, Pechini, sonochemical, precipitation, solid-state, and pulsed-laser-induced methods (Culver *et al.*, 2013; Lei & Yan, 2008; Wang *et al.*, 2006; Kodaira *et al.*, 2003; Geng *et al.*, 2006; Ahmad *et al.*, 2006; Ryu *et al.*, 2007). The sizes and morphologies of the scheelite-structured crystals are important for specific applications and were controlled under some of these methods. Culver *et al.* (2013) successfully synthesized < 30 nm $AMoO_4$ (A = Ca, Sr, Ba) crystals using the VDSG method for Li-ion battery electrodes. Lei & Yan (2008) showed different sizes (30–40 nm) of $CaMO_4$:RE (M = W, Mo; RE = Eu, Tb) by varying the synthesis temperature (120–220°C) of hydrothermal experiments. Geng *et al.* (2006) used a sonochemical method with varying pH to synthesize $PbWO_4$ with different morphologies.

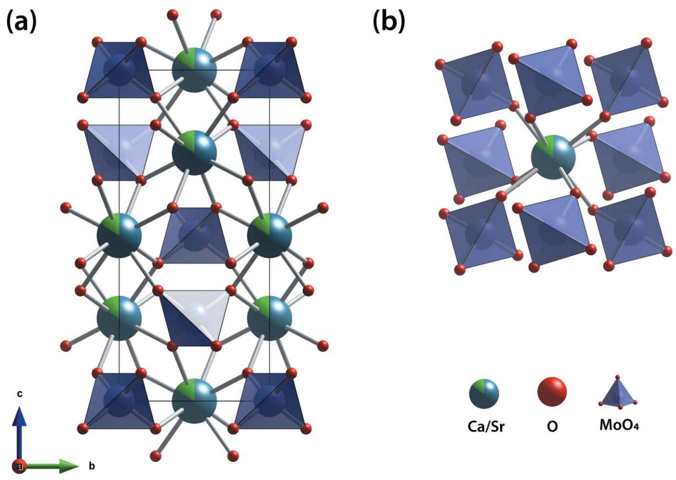


Figure 1
(a) Crystal structure of $Ca_{0.84}Sr_{0.16}MoO_4$ and (b) coordination of eight $[MoO_4]^{2-}$ tetrahedra with respect to the Ca/Sr cations.

Ryu *et al.* (2007) used the pulsed-laser ablation method to synthesize spherical powellite particles of 16–29 nm.

2. Structural commentary

Powellite crystallizes in the tetragonal space group $I4_1/a$ and contains Ca^{2+} cations coordinated by eight $[MoO_4]^{2-}$ tetrahedra, sharing an oxygen atom with each tetrahedron. The crystal structure of $Ca_{0.84}Sr_{0.16}MoO_4$ is isostructural to powellite, but with larger unit-cell parameters and (Ca/Sr)—O bond distances compared to $CaMoO_4$ powellite because of the partial incorporation of the larger Sr^{2+} cation into the Ca^{2+} sites (Fig. 1). Similarly, the Ba—O and Sr—O bond distances in $BaMoO_4$ (Nassif *et al.*, 1999; Panchal *et al.*, 2006; Cavalcante *et al.*, 2008) and $SrMoO_4$ (Egorov-Tismenko *et al.*, 1967; Gürmen *et al.*, 1971; Nogueira *et al.*, 2013) are longer than the Ca—O bond distance in $CaMoO_4$ (Aleksandrov *et al.*, 1968; Gürmen *et al.*, 1971) or the (Ca/Sr)—O bond distance in this study. Fig. 2 shows a summary of unit-cell parameters (a and c), unit-cell volumes (V), and unit-cell densities (ρ) from the literature as well as the current composition including $CaMoO_4$ (Aleksandrov *et al.*, 1968; Gürmen *et al.*, 1971; Wandahl & Christensen, 1987; Peterson *et al.*, 2018), $Ca_{0.747}Sr_{0.194}Ba_{0.059}MoO_4$ (Peterson *et al.*, 2018), $SrMoO_4$ (Gürmen *et al.*, 1971; Egorov-Tismenko *et al.*, 1967; Nogueira *et al.*, 2013; Peterson *et al.*, 2018), $Sr_{0.81}Ba_{0.19}MoO_4$ (Nogueira *et al.*, 2013), $Sr_{0.59}Ba_{0.41}MoO_4$ (Nogueira *et al.*, 2013), $Ca_{0.088}Sr_{0.256}Ba_{0.656}MoO_4$ (Peterson *et al.*, 2018), $Sr_{0.27}Ba_{0.73}MoO_4$ (Nogueira *et al.*, 2013), and $BaMoO_4$ (Cavalcante *et al.*, 2008; Panchal *et al.*, 2006; Vegard & Refsum, 1927; Nogueira *et al.*, 2013; Nassif *et al.*, 1999; Bylichkina *et al.*, 1970; Peterson *et al.*, 2018). The structural parameters of $Ca_{0.84}Sr_{0.16}MoO_4$ fit well to the trendlines in Fig. 2, and the data show well-fit linear relationships for the unit cell and volume. For the density, a non-linear trendline was drawn based on the densities of end members, and a linear trendline was drawn using the densities from both end members and

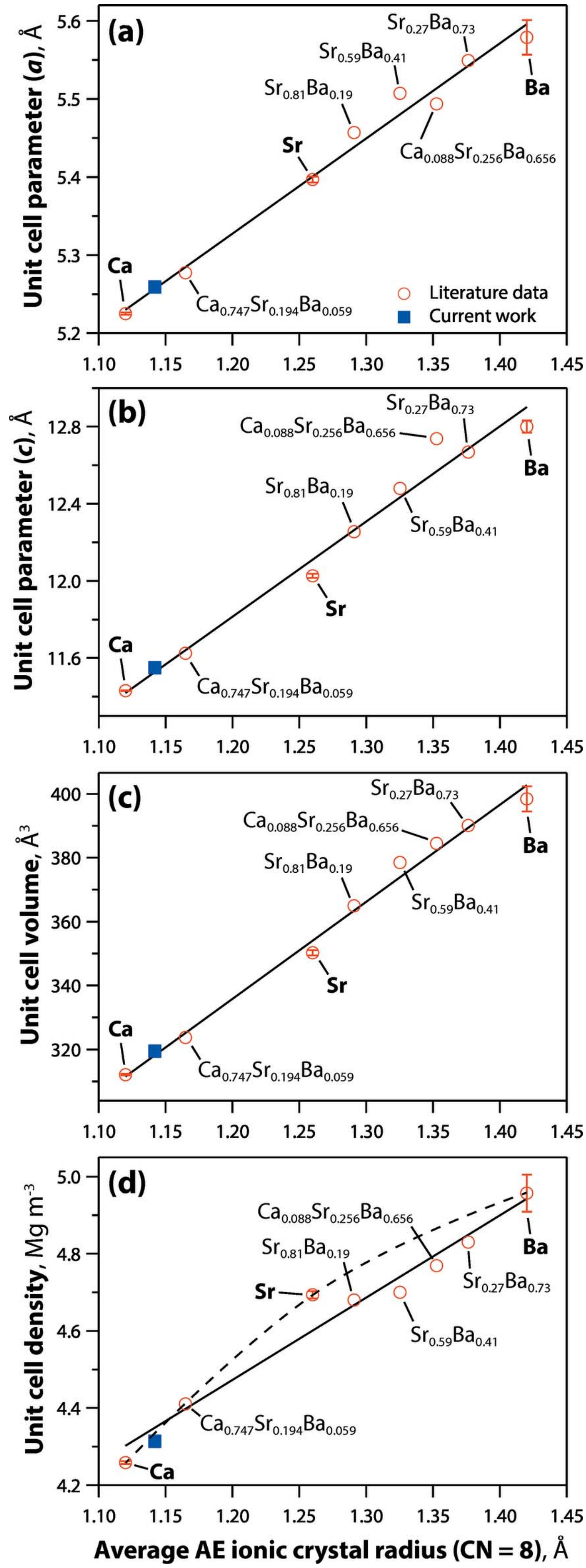


Figure 2
Summary of (a) unit-cell parameter a, (b) unit-cell parameter c, (c) unit-cell volume (V), and (d) density (ρ) as a function of the average ionic crystal radii in the structure (coordination number = 8) from Shannon (1976). Data for the end members include averages and standard deviations from multiple sources.

Table 1
Summary of data on (Ca, Sr, Ba)MoO_4 crystals from the literature and current study.

Densities are calculated from crystallographic data.

Chemistry	*a* (Å)	*c* (Å)	Volume (Å^3)	Density (Mg m^{-3})	Reference
$CaMoO_4$	5.224	11.43	311.93	4.26	(Aleksandrov *et al.*, 1968)
$CaMoO_4$	5.224	11.43	312.17	4.26	(Gürmen *et al.*, 1971)
$CaMoO_4$	5.2235	11.4298	311.86	4.26	(Wandahl & Christensen, 1987)
$CaMoO_4$	5.2268	11.4345	312.38	4.25	(Peterson *et al.*, 2018)
$Ca_{0.84}Sr_{0.16}MoO_4$	5.2592	11.5500	319.45	4.32	Current study
$SrMoO_4$	5.394	12.017	349.64	4.7	(Egorov-Tismenko *et al.*, 1967)
$SrMoO_4$	5.3944	12.02	349.78	4.7	(Gürmen *et al.*, 1971)
$SrMoO_4$	5.4026	12.0411	351.46	4.68	(Nogueira *et al.*, 2013)
$SrMoO_4$	5.3963	12.0248	350.16	4.7	(Peterson *et al.*, 2018)
$Sr_{0.81}Ba_{0.19}MoO_4$	5.4571	12.2548	364.95	4.68	(Nogueira *et al.*, 2013)
$Sr_{0.59}Ba_{0.41}MoO_4$	5.5073	12.4789	378.49	4.7	(Nogueira *et al.*, 2013)
$Sr_{0.27}Ba_{0.73}MoO_4$	5.5491	12.6680	390.08	4.83	(Nogueira *et al.*, 2013)
$BaMoO_4$	5.567	12.78	396.07	4.99	(Vegard & Refsum, 1927)
$BaMoO_4$	5.62	12.82	404.91	4.88	(Bylichkina *et al.*, 1970)
$BaMoO_4$	5.5479	12.743	392.22	5.03	(Nassif *et al.*, 1999)
$BaMoO_4$	5.5800	12.820	399.17	4.95	(Panchal *et al.*, 2006)
$BaMoO_4$	5.5696	12.7865	396.64	4.98	(Cavalcante *et al.*, 2008)
$BaMoO_4$	5.5848	12.8292	400.15	4.93	(Nogueira *et al.*, 2013)
$BaMoO_4$	5.5828	12.8204	399.59	4.94	(Peterson *et al.*, 2018)

mixed powellites from the literature (Fig. 2*d*). Despite our expectation, the density values did not fit well into either trendline, and more density values from different chemistries of mixed alkaline-earth powellites would help to understand the behavior of densities in powellites. The trendlines show that the unit cells, volumes, and densities all increase with larger alkaline-earth cations. Details of unit cell parameters, volumes, and densities from literature and the current study are summarized in Table 1.

3. Synthesis and crystallization

The mixed alkaline-earth powellite, $Ca_{0.84}Sr_{0.16}MoO_4$, was synthesized using the end-member powellites within a LiCl flux. The loss of mass due to dehydration for LiCl was measured by placing a given amount of LiCl (Alfa Aesar, >99%) into a furnace at 100°C and weighing daily for five days. For the synthesis of $CaMoO_4$ and $SrMoO_4$, the stoichiometric amounts of $CaCO_3$ (Alfa Aesar, >99.5%), $SrCO_3$ (Sigma Aldrich, >99.9%), and MoO_3 (Alfa Aesar, >99.5%) were placed in Pt/10%Rh crucible and heated to 1500°C at 5°C min^{-1}, held for 30 min, ramped down to 1400°C at 1°C min^{-1}, held for 1 h, and then cooled down to room temperature at 1°C min^{-1}. Details of synthesis are provided elsewhere (Peterson *et al.*, 2018). For the synthesis of $Ca_{0.84}Sr_{0.16}MoO_4$, appropriate amounts of $CaMoO_4$ and $SrMoO_4$ powders were used as precursors and mixed together in Pt/10%Rh crucibles. Then, LiCl was added at a 1:1 ratio by mass, where the mass of $CaMoO_4$ + $SrMoO_4$ was equivalent to that of the LiCl. The crucible was covered with a tight-fitting Pt/10%Rh lid and heated according to a method described by Arora *et al.* (1983). The furnace was ramped up to 850°C, held for 2 h, abruptly decreased to 750°C, cooled to 550°C at a rate of 3°C h^{-1}, and then the furnace was shut off. Crystals were recovered after washing in a sonic bath and rinsing with deionized water.

4. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. For the occupancy refinement of the Ca and Sr sites, the occupancy parameters of both Sr and Ca were refined with isotropic atomic displacement parameters while keeping the total occupancy as 1. The refined occupancy values were 0.86 for Ca and 0.14 for Sr after rounding, and then these values were fixed and anisotropic refinements were performed on all the atoms including Ca, Sr, Mo, and O. The final refinement converged at R_1 = 4.30%, and the goodness-of-fit was 1.44. The single crystals of $Ca_{0.84}Sr_{0.16}MoO_4$ were ground with a mortar and pestle. A selected crystal for SC-XRD was placed on a cryoloop in oil

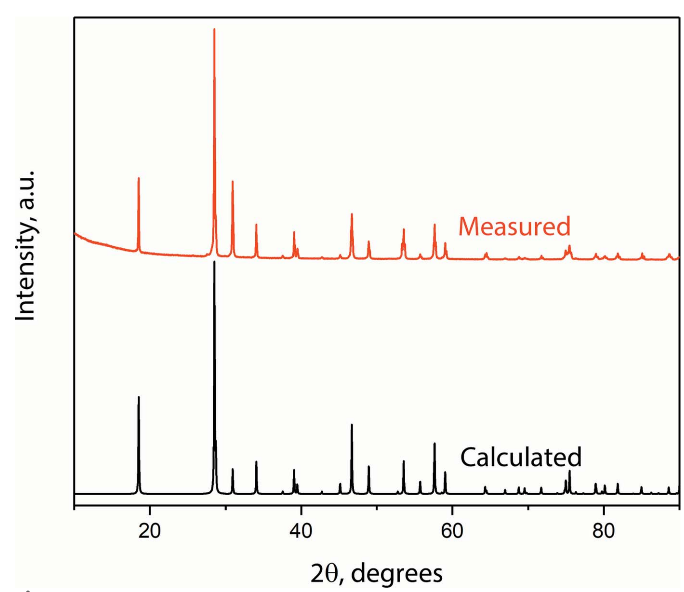


Figure 3
Comparison between P-XRD pattern of ground $Ca_{0.84}Sr_{0.16}MoO_4$ single crystals and calculated pattern generated from the solved structure.

Table 2
Experimental details.

Crystal data	
Chemical formula	$Ca_{0.84}Sr_{0.16}MoO_4$
M_r	207.6
Crystal system, space group	Tetragonal, $I4_1/a$
Temperature (K)	293
a, c (Å)	5.2592 (1), 11.5497 (4)
V (Å^3)	319.46 (1)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.92
Crystal size (mm)	0.05 × 0.05 × 0.03
Data collection	
Diffractometer	Bruker D8 QUEST CMOS area detector
Absorption correction	Multi-scan (*SADABS*)
T_{min}, T_{max}	0.628, 0.747
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6597, 396, 238
R_{int}	0.131
Refinement	
$R[F > 3\sigma(F)]$, $wR(F)$, S	0.043, 0.042, 1.44
No. of reflections	396
No. of parameters	14
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.76, −2.57

Computer programs: *APEX3* and *SAINT* (Bruker, 2012), *JANA2006* (Petříček *et al.*, 2014), *SUPERFLIP* (Palatinus & Chapuis, 2007), *VESTA* (Momma & Izumi, 2011), *publCIF* (Westrip, 2010).

(Parabar 10312, Hampton Research). Powder X-ray diffraction (P-XRD) was performed using a Bruker D8 Advance diffractometer on a zero-background quartz sample holder. The measured P-XRD pattern was compared to the calculated pattern from the solved structure, and they were in good agreement (see Fig. 3).

Acknowledgements

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References

Ahmad, G., Dickerson, M. B., Church, B. C., Cai, Y., Jones, S. E., Naik, R. R., King, J. S., Summers, C. J., Kröger, N. & Sandhage, K. H. (2006). *Adv. Mater.* **18**, 1759–1763.
Aleksandrov, V. B., Gorbatyii, L. V. & Ilyukhin, V. V. (1968). *Kristallografiya*, **13**, 512–513.
Arora, S. K., Godbole, R. S. & Rao, G. S. T. (1983). *J. Am. Ceram. Soc.* **66**, 321–323.
Bi, J., Cui, C.-H., Lai, X., Shi, F. & Gao, D.-J. (2008). *Mater. Res. Bull.* **43**, 743–747.
Bruker (2012). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bylichkina, T. I., Soleva, L. I., Pobedimskaya, E. A., Porai Koshits, M. A. & Belov, N. V. (1970). *Kristallografiya*, **15**, 165–167.
Cavalcante, L. S., Sczancoski, J. C., Tranquilin, R. L., Joya, M. R., Pizani, P. S., Varela, J. A. & Longo, E. (2008). *J. Phys. Chem. Solids*, **69**, 2674–2680.
Crum, J. V., Chong, S., Peterson, J. A. & Riley, B. J. (2019). *Acta Cryst.* E**75**, 1020–1025.
Culver, S. P., Rabuffetti, F. A., Zhou, S., Mecklenburg, M., Song, Y., Melot, B. C. & Brutchey, R. L. (2013). *Chem. Mater.* **25**, 4129–4134.
Egorov-Tismenko, Y. K., Simonov, M. A. & Belov, N. V. (1967). *Kristallografiya*, **12**, 511–512.
Geng, J., Zhu, J.-J. & Chen, H.-Y. (2006). *Cryst. Growth Des.* **6**, 321–326.
Gürmen, E., Daniels, E. & King, J. S. (1971). *J. Chem. Phys.* **55**, 1093–1097.
Kato, A., Oishi, S., Shishido, T., Yamazaki, M. & Iida, S. (2005). *J. Phys. Chem. Solids*, **66**, 2079–2081.
Kim, T. & Kang, S. (2007). *J. Lumin.* **122–123**, 964–966.
Kodaira, C. A., Brito, H. F. & Felinto, M. C. F. C. (2003). *J. Solid State Chem.* **171**, 401–407.
Lei, F. & Yan, B. (2008). *J. Solid State Chem.* **181**, 855–862.
Lei, H., Zhang, S., Zhu, X., Sun, Y. & Fu, Y. (2010). *Mater. Lett.* **64**, 344–346.
Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
Nassif, V., Carbonio, R. E. & Alonso, J. A. (1999). *J. Solid State Chem.* **146**, 266–270.
Nogueira, I. C., Cavalcante, L. S., Pereira, P. F. S., de Jesus, M. M., Rivas Mercury, J. M., Batista, N. C., Li, M. S. & Longo, E. (2013). *J. Appl. Cryst.* **46**, 1434–1446.
Palatinus, L. & Chapuis, G. (2007). *J. Appl. Cryst.* **40**, 786–790.
Panchal, V., Garg, N. & Sharma, S. M. (2006). *J. Phys. Condens. Matter*, **18**, 3917–3929.
Peterson, J. A., Crum, J. V., Riley, B. J., Asmussen, R. M. & Neeway, J. J. (2018). *J. Nucl. Mater.* **510**, 623–634.
Petříček, V., Dusek, M. & Palatinus, L. (2014). *Z. Kristallogr.* **229**, 345–352.
Rabuffetti, F. A., Culver, S. P., Suescun, L. & Brutchey, R. L. (2014). *Inorg. Chem.* **53**, 1056–1061.
Reddy, M., Subba Rao, G. V. & Chowdari, B. V. R. (2013). *Chem. Rev.* **113**, 5364–5457.
Ryu, J. H., Bang, S. Y., Yoon, J.-W., Lim, C. S. & Shim, K. B. (2007). *Appl. Surf. Sci.* **253**, 8408–8414.
Schmidt, M., Heck, S., Bosbach, D., Ganschow, S., Walther, C. & Stumpf, T. (2013). *Dalton Trans.* **42**, 8387–8393.
Shannon, R. D. (1976). *Acta Cryst.* A**32**, 751–767.
Vegard, L. & Refsum, A. (1927). *Skrifter utgitt av det Norske Videnskaps-Akademi i Oslo 1: Matematisk-Naturvidenskapelig Klasse*, 1.
Wandahl, G. & Christensen, A. N. (1987). *Acta Chem. Scand.* **41**, 358–360.
Wang, Y., Ma, J., Tao, J., Zhu, X., Zhou, J., Zhao, Z., Xie, L. & Tian, H. (2006). *Mater. Lett.* **60**, 291–293.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

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Synthesis and crystal structure of a mixed alkaline-earth powellite, $Ca_{0.84}Sr_{0.16}MoO_4$

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Computing details

Data collection: *APEX3* (Bruker, 2012); cell refinement: JANA2006 (Petříček *et al.*, 2014); data reduction: *SAINT* (Bruker, 2012); program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: JANA2006 (Petříček *et al.*, 2014); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Calcium strontium molybdate

Crystal data

$Ca_{0.84}Sr_{0.16}MoO_4$
M_r = 207.6
Tetragonal, $I4_1/a$:1
Hall symbol: I 4bw -1bw
a = 5.2592 (1) Å
c = 11.5497 (4) Å
V = 319.46 (1) $Å^3$
Z = 4
F(000) = 388
D_x = 4.317 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 6597 reflections
θ = 4.3–36.5°
μ = 7.92 mm^{-1}
T = 293 K
Irregular, light white
0.05 × 0.05 × 0.03 mm

Data collection

Bruker D8 QUEST CMOS area detector diffractometer
Radiation source: X-ray tube
φ and ω scans
Absorption correction: multi-scan (SADABS)
T_{min} = 0.628, T_{max} = 0.747
6597 measured reflections
396 independent reflections
238 reflections with $I > 2\sigma(I)$
R_{int} = 0.131
θ_{max} = 36.5°, θ_{min} = 4.3°
h = −8→8
k = −8→8
l = −19→19

Refinement

Refinement on F
$R[F > 3\sigma(F)]$ = 0.043
$wR(F)$ = 0.042
S = 1.44
396 reflections
14 parameters
0 restraints
2 constraints
Primary atom site location: iterative
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(F) + 0.0001F^2)$
$(\Delta/\sigma)_{max}$ = 0.024
$\Delta\rho_{max}$ = 2.76 e $Å^{-3}$
$\Delta\rho_{min}$ = −2.57 e $Å^{-3}$

Special details

Refinement. F000 reported from JANA is 388.0 and calculated is 387.5 from CheckCIF.Both occupancies of Ca and Sr were refined with isotropic ADP while keeping the total occupancy at 1 and same position for both atoms, and their occupancy values were closed to 0.84 ±0.001 and 0.16±0.001 respectively between the refinements. Therefore, we fixed the occupancy to 0.84 and 0.16 with rounding off, and the anisotropic refinement was applied after fixing the occupancies.The difference in reported and caculated rho(max)is likely due to difference in how PLATON and JANA2006 calculate Fourier maps and take weights of reflections into Fourier calculations.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.5	0.5	0	0.00778 (13)	
Ca1	1	0.5	0.25	0.0074 (2)	0.84
Sr1	1	0.5	0.25	0.0074 (2)	0.16
O1	0.7420 (7)	0.6444 (7)	0.0837 (3)	0.0114 (8)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0067 (2)	0.0067 (2)	0.0100 (2)	0	0	0
Ca1	0.0076 (4)	0.0076 (4)	0.0072 (4)	0	0	0
Sr1	0.0076 (4)	0.0076 (4)	0.0072 (4)	0	0	0
O1	0.0127 (17)	0.0088 (16)	0.0126 (10)	−0.0017 (14)	−0.0039 (12)	0.0016 (11)

Geometric parameters (Å, º)

Mo1—Sr1^{i}	3.7188	Ca1—Sr1^{iii}	3.9054
Mo1—Sr1^{ii}	3.7188	Ca1—Sr1^{iv}	3.9054
Mo1—Sr1^{iii}	3.7188	Sr1—Sr1^{viii}	3.9054
Mo1—Sr1^{iv}	3.7188	Sr1—Sr1^{ix}	3.9054
Mo1—O1	1.769 (3)	Sr1—Sr1^{iii}	3.9054
Mo1—O1^{v}	1.769 (3)	Sr1—Sr1^{iv}	3.9054
Mo1—O1^{vi}	1.769 (3)	Sr1—O1	2.471 (3)
Mo1—O1^{vii}	1.769 (3)	Sr1—O1^{x}	2.471 (3)
Ca1—Ca1^{viii}	3.9054	Sr1—O1^{ix}	2.505 (4)
Ca1—Ca1^{ix}	3.9054	Sr1—O1^{xi}	2.505 (4)
Ca1—Ca1^{iii}	3.9054	Sr1—O1^{xii}	2.505 (4)
Ca1—Ca1^{iv}	3.9054	Sr1—O1^{xiii}	2.505 (4)
Ca1—Sr1	0	Sr1—O1^{xiv}	2.471 (3)
Ca1—Sr1^{viii}	3.9054	Sr1—O1^{xv}	2.471 (3)
Ca1—Sr1^{ix}	3.9054		
Sr1^{i}—Mo1—Sr1^{ii}	90	Ca1—Sr1—Ca1^{ix}	0
Sr1^{i}—Mo1—Sr1^{iii}	90	Ca1—Sr1—Ca1^{iii}	0
Sr1^{i}—Mo1—Sr1^{iv}	180.0 (5)	Ca1—Sr1—Ca1^{iv}	0
Sr1^{i}—Mo1—O1	144.30 (11)	Ca1—Sr1—Sr1^{viii}	0
Sr1^{i}—Mo1—O1^{v}	35.70 (11)	Ca1—Sr1—Sr1^{ix}	0
Sr1^{i}—Mo1—O1^{vi}	78.16 (12)	Ca1—Sr1—Sr1^{iii}	0
Sr1^{i}—Mo1—O1^{vii}	101.84 (12)	Ca1—Sr1—Sr1^{iv}	0

Sr1ii—Mo1—Sr1iii	180.0 (5)	Ca1—Sr1—O1	0
Sr1ii—Mo1—Sr1iv	90	Ca1—Sr1—O1x	0
Sr1ii—Mo1—O1	101.84 (12)	Ca1—Sr1—O1ix	0
Sr1ii—Mo1—O1v	78.16 (12)	Ca1—Sr1—O1xi	0
Sr1ii—Mo1—O1vi	144.30 (11)	Ca1—Sr1—O1xii	0
Sr1ii—Mo1—O1vii	35.70 (11)	Ca1—Sr1—O1xiii	0
Sr1iii—Mo1—Sr1iv	90	Ca1—Sr1—O1xiv	0
Sr1iii—Mo1—O1	78.16 (12)	Ca1—Sr1—O1xv	0
Sr1iii—Mo1—O1v	101.84 (12)	Ca1viii—Sr1—Ca1ix	84.65
Sr1iii—Mo1—O1vi	35.70 (11)	Ca1viii—Sr1—Ca1iii	123.14
Sr1iii—Mo1—O1vii	144.30 (11)	Ca1viii—Sr1—Ca1iv	123.14
Sr1iv—Mo1—O1	35.70 (11)	Ca1viii—Sr1—Sr1viii	0.0 (5)
Sr1iv—Mo1—O1v	144.30 (11)	Ca1viii—Sr1—Sr1ix	84.65
Sr1iv—Mo1—O1vi	101.84 (12)	Ca1viii—Sr1—Sr1iii	123.14
Sr1iv—Mo1—O1vii	78.16 (12)	Ca1viii—Sr1—Sr1iv	123.14
O1—Mo1—O1v	113.77 (15)	Ca1viii—Sr1—O1	101.82 (8)
O1—Mo1—O1vi	107.37 (16)	Ca1viii—Sr1—O1x	160.80 (8)
O1—Mo1—O1vii	107.37 (16)	Ca1viii—Sr1—O1ix	102.56 (7)
O1v—Mo1—O1vi	107.37 (16)	Ca1viii—Sr1—O1xi	37.99 (8)
O1v—Mo1—O1vii	107.37 (16)	Ca1viii—Sr1—O1xii	130.55 (8)
O1vi—Mo1—O1vii	113.77 (15)	Ca1viii—Sr1—O1xiii	85.44 (8)
Ca1viii—Ca1—Ca1ix	84.65	Ca1viii—Sr1—O1xiv	68.42 (8)
Ca1viii—Ca1—Ca1iii	123.14	Ca1viii—Sr1—O1xv	38.60 (8)
Ca1viii—Ca1—Ca1iv	123.14	Ca1ix—Sr1—Ca1iii	123.14
Ca1viii—Ca1—Sr1	0	Ca1ix—Sr1—Ca1iv	123.14
Ca1viii—Ca1—Sr1viii	0.0 (5)	Ca1ix—Sr1—Sr1viii	84.65
Ca1viii—Ca1—Sr1ix	84.65	Ca1ix—Sr1—Sr1ix	0.0 (5)
Ca1viii—Ca1—Sr1iii	123.14	Ca1ix—Sr1—Sr1iii	123.14
Ca1viii—Ca1—Sr1iv	123.14	Ca1ix—Sr1—Sr1iv	123.14
Ca1ix—Ca1—Ca1iii	123.14	Ca1ix—Sr1—O1	160.80 (8)
Ca1ix—Ca1—Ca1iv	123.14	Ca1ix—Sr1—O1x	101.82 (8)
Ca1ix—Ca1—Sr1	0	Ca1ix—Sr1—O1ix	37.99 (8)
Ca1ix—Ca1—Sr1viii	84.65	Ca1ix—Sr1—O1xi	102.56 (7)
Ca1ix—Ca1—Sr1ix	0.0 (5)	Ca1ix—Sr1—O1xii	85.44 (8)
Ca1ix—Ca1—Sr1iii	123.14	Ca1ix—Sr1—O1xiii	130.55 (8)
Ca1ix—Ca1—Sr1iv	123.14	Ca1ix—Sr1—O1xiv	38.60 (8)
Ca1iii—Ca1—Ca1iv	84.65	Ca1ix—Sr1—O1xv	68.42 (8)
Ca1iii—Ca1—Sr1	0	Ca1iii—Sr1—Ca1iv	84.65
Ca1iii—Ca1—Sr1viii	123.14	Ca1iii—Sr1—Sr1viii	123.14
Ca1iii—Ca1—Sr1ix	123.14	Ca1iii—Sr1—Sr1ix	123.14
Ca1iii—Ca1—Sr1iii	0.0 (5)	Ca1iii—Sr1—Sr1iii	0.0 (5)
Ca1iii—Ca1—Sr1iv	84.65	Ca1iii—Sr1—Sr1iv	84.65
Ca1iv—Ca1—Sr1	0	Ca1iii—Sr1—O1	68.42 (8)
Ca1iv—Ca1—Sr1viii	123.14	Ca1iii—Sr1—O1x	38.60 (8)
Ca1iv—Ca1—Sr1ix	123.14	Ca1iii—Sr1—O1ix	85.44 (8)
Ca1iv—Ca1—Sr1iii	84.65	Ca1iii—Sr1—O1xi	130.55 (8)
Ca1iv—Ca1—Sr1iv	0.0 (5)	Ca1iii—Sr1—O1xii	102.56 (7)
Sr1—Ca1—Sr1viii	0	Ca1iii—Sr1—O1xiii	37.99 (8)

Sr1—Ca1—Sr1^{ix}	0	Ca1^{iii}—Sr1—O1^{xiv}	160.80 (8)
Sr1—Ca1—Sr1^{iii}	0	Ca1^{iii}—Sr1—O1^{xv}	101.82 (8)
Sr1—Ca1—Sr1^{iv}	0	Ca1^{iv}—Sr1—Sr1^{viii}	123.14
Sr1^{viii}—Ca1—Sr1^{ix}	84.65	Ca1^{iv}—Sr1—Sr1^{ix}	123.14
Sr1^{viii}—Ca1—Sr1^{iii}	123.14	Ca1^{iv}—Sr1—Sr1^{iii}	84.65
Sr1^{viii}—Ca1—Sr1^{iv}	123.14	Ca1^{iv}—Sr1—Sr1^{iv}	0.0 (5)
Sr1^{ix}—Ca1—Sr1^{iii}	123.14	Ca1^{iv}—Sr1—O1	38.60 (8)
Sr1^{ix}—Ca1—Sr1^{iv}	123.14	Ca1^{iv}—Sr1—O1^{x}	68.42 (8)
Sr1^{iii}—Ca1—Sr1^{iv}	84.65	Ca1^{iv}—Sr1—O1^{ix}	130.55 (8)
Mo1^{viii}—Sr1—Mo1^{xvi}	90	Ca1^{iv}—Sr1—O1^{xi}	85.44 (8)
Mo1^{viii}—Sr1—Mo1^{ix}	90	Ca1^{iv}—Sr1—O1^{xii}	37.99 (8)
Mo1^{viii}—Sr1—Mo1^{xvii}	180.0 (5)	Ca1^{iv}—Sr1—O1^{xiii}	102.56 (7)
Mo1^{viii}—Sr1—Ca1	0	Ca1^{iv}—Sr1—O1^{xiv}	101.82 (8)
Mo1^{viii}—Sr1—Ca1^{viii}	61.57	Ca1^{iv}—Sr1—O1^{xv}	160.80 (8)
Mo1^{viii}—Sr1—Ca1^{ix}	118.43	Sr1^{viii}—Sr1—Sr1^{ix}	84.65
Mo1^{viii}—Sr1—Ca1^{iii}	61.57	Sr1^{viii}—Sr1—Sr1^{iii}	123.14
Mo1^{viii}—Sr1—Ca1^{iv}	118.43	Sr1^{viii}—Sr1—Sr1^{iv}	123.14
Mo1^{viii}—Sr1—Sr1^{viii}	61.57	Sr1^{viii}—Sr1—O1	101.82 (8)
Mo1^{viii}—Sr1—Sr1^{ix}	118.43	Sr1^{viii}—Sr1—O1^{x}	160.80 (8)
Mo1^{viii}—Sr1—Sr1^{iii}	61.57	Sr1^{viii}—Sr1—O1^{ix}	102.56 (7)
Mo1^{viii}—Sr1—Sr1^{iv}	118.43	Sr1^{viii}—Sr1—O1^{xi}	37.99 (8)
Mo1^{viii}—Sr1—O1	80.15 (8)	Sr1^{viii}—Sr1—O1^{xii}	130.55 (8)
Mo1^{viii}—Sr1—O1^{x}	99.85 (8)	Sr1^{viii}—Sr1—O1^{xiii}	85.44 (8)
Mo1^{viii}—Sr1—O1^{ix}	98.33 (8)	Sr1^{viii}—Sr1—O1^{xiv}	68.42 (8)
Mo1^{viii}—Sr1—O1^{xi}	81.67 (8)	Sr1^{viii}—Sr1—O1^{xv}	38.60 (8)
Mo1^{viii}—Sr1—O1^{xii}	155.66 (7)	Sr1^{ix}—Sr1—Sr1^{iii}	123.14
Mo1^{viii}—Sr1—O1^{xiii}	24.34 (7)	Sr1^{ix}—Sr1—Sr1^{iv}	123.14
Mo1^{viii}—Sr1—O1^{xiv}	127.27 (8)	Sr1^{ix}—Sr1—O1	160.80 (8)
Mo1^{viii}—Sr1—O1^{xv}	52.73 (8)	Sr1^{ix}—Sr1—O1^{x}	101.82 (8)
Mo1^{xvi}—Sr1—Mo1^{ix}	180.0 (5)	Sr1^{ix}—Sr1—O1^{ix}	37.99 (8)
Mo1^{xvi}—Sr1—Mo1^{xvii}	90	Sr1^{ix}—Sr1—O1^{xi}	102.56 (7)
Mo1^{xvi}—Sr1—Ca1	0	Sr1^{ix}—Sr1—O1^{xii}	85.44 (8)
Mo1^{xvi}—Sr1—Ca1^{viii}	61.57	Sr1^{ix}—Sr1—O1^{xiii}	130.55 (8)
Mo1^{xvi}—Sr1—Ca1^{ix}	118.43	Sr1^{ix}—Sr1—O1^{xiv}	38.60 (8)
Mo1^{xvi}—Sr1—Ca1^{iii}	118.43	Sr1^{ix}—Sr1—O1^{xv}	68.42 (8)
Mo1^{xvi}—Sr1—Ca1^{iv}	61.57	Sr1^{iii}—Sr1—Sr1^{iv}	84.65
Mo1^{xvi}—Sr1—Sr1^{viii}	61.57	Sr1^{iii}—Sr1—O1	68.42 (8)
Mo1^{xvi}—Sr1—Sr1^{ix}	118.43	Sr1^{iii}—Sr1—O1^{x}	38.60 (8)
Mo1^{xvi}—Sr1—Sr1^{iii}	118.43	Sr1^{iii}—Sr1—O1^{ix}	85.44 (8)
Mo1^{xvi}—Sr1—Sr1^{iv}	61.57	Sr1^{iii}—Sr1—O1^{xi}	130.55 (8)
Mo1^{xvi}—Sr1—O1	52.73 (8)	Sr1^{iii}—Sr1—O1^{xii}	102.56 (7)
Mo1^{xvi}—Sr1—O1^{x}	127.27 (8)	Sr1^{iii}—Sr1—O1^{xiii}	37.99 (8)
Mo1^{xvi}—Sr1—O1^{ix}	155.66 (7)	Sr1^{iii}—Sr1—O1^{xiv}	160.80 (8)
Mo1^{xvi}—Sr1—O1^{xi}	24.34 (7)	Sr1^{iii}—Sr1—O1^{xv}	101.82 (8)
Mo1^{xvi}—Sr1—O1^{xii}	81.67 (8)	Sr1^{iv}—Sr1—O1	38.60 (8)
Mo1^{xvi}—Sr1—O1^{xiii}	98.33 (8)	Sr1^{iv}—Sr1—O1^{x}	68.42 (8)
Mo1^{xvi}—Sr1—O1^{xiv}	80.15 (8)	Sr1^{iv}—Sr1—O1^{ix}	130.55 (8)
Mo1^{xvi}—Sr1—O1^{xv}	99.85 (8)	Sr1^{iv}—Sr1—O1^{xi}	85.44 (8)

$Mo1^{ix}—Sr1—Mo1^{xvii}$	90	$Sr1^{iv}—Sr1—O1^{xii}$	37.99 (8)
$Mo1^{ix}—Sr1—Ca1$	0	$Sr1^{iv}—Sr1—O1^{xiii}$	102.56 (7)
$Mo1^{ix}—Sr1—Ca1^{viii}$	118.43	$Sr1^{iv}—Sr1—O1^{xiv}$	101.82 (8)
$Mo1^{ix}—Sr1—Ca1^{ix}$	61.57	$Sr1^{iv}—Sr1—O1^{xv}$	160.80 (8)
$Mo1^{ix}—Sr1—Ca1^{iii}$	61.57	$O1—Sr1—O1^{x}$	77.98 (11)
$Mo1^{ix}—Sr1—Ca1^{iv}$	118.43	$O1—Sr1—O1^{ix}$	151.21 (11)
$Mo1^{ix}—Sr1—Sr1^{viii}$	118.43	$O1—Sr1—O1^{xi}$	73.95 (11)
$Mo1^{ix}—Sr1—Sr1^{ix}$	61.57	$O1—Sr1—O1^{xii}$	76.60 (11)
$Mo1^{ix}—Sr1—Sr1^{iii}$	61.57	$O1—Sr1—O1^{xiii}$	68.41 (11)
$Mo1^{ix}—Sr1—Sr1^{iv}$	118.43	$O1—Sr1—O1^{xiv}$	127.16 (12)
$Mo1^{ix}—Sr1—O1$	127.27 (8)	$O1—Sr1—O1^{xv}$	127.16 (12)
$Mo1^{ix}—Sr1—O1^{x}$	52.73 (8)	$O1^{x}—Sr1—O1^{ix}$	73.95 (11)
$Mo1^{ix}—Sr1—O1^{ix}$	24.34 (7)	$O1^{x}—Sr1—O1^{xi}$	151.21 (11)
$Mo1^{ix}—Sr1—O1^{xi}$	155.66 (7)	$O1^{x}—Sr1—O1^{xii}$	68.41 (11)
$Mo1^{ix}—Sr1—O1^{xii}$	98.33 (8)	$O1^{x}—Sr1—O1^{xiii}$	76.60 (11)
$Mo1^{ix}—Sr1—O1^{xiii}$	81.67 (8)	$O1^{x}—Sr1—O1^{xiv}$	127.16 (12)
$Mo1^{ix}—Sr1—O1^{xiv}$	99.85 (8)	$O1^{x}—Sr1—O1^{xv}$	127.16 (12)
$Mo1^{ix}—Sr1—O1^{xv}$	80.15 (8)	$O1^{ix}—Sr1—O1^{xi}$	134.61 (10)
$Mo1^{xvii}—Sr1—Ca1$	0	$O1^{ix}—Sr1—O1^{xii}$	98.56 (12)
$Mo1^{xvii}—Sr1—Ca1^{viii}$	118.43	$O1^{ix}—Sr1—O1^{xiii}$	98.56 (12)
$Mo1^{xvii}—Sr1—Ca1^{ix}$	61.57	$O1^{ix}—Sr1—O1^{xiv}$	76.60 (11)
$Mo1^{xvii}—Sr1—Ca1^{iii}$	118.43	$O1^{ix}—Sr1—O1^{xv}$	68.41 (11)
$Mo1^{xvii}—Sr1—Ca1^{iv}$	61.57	$O1^{xi}—Sr1—O1^{xii}$	98.56 (12)
$Mo1^{xvii}—Sr1—Sr1^{viii}$	118.43	$O1^{xi}—Sr1—O1^{xiii}$	98.56 (12)
$Mo1^{xvii}—Sr1—Sr1^{ix}$	61.57	$O1^{xi}—Sr1—O1^{xiv}$	68.41 (11)
$Mo1^{xvii}—Sr1—Sr1^{iii}$	118.43	$O1^{xi}—Sr1—O1^{xv}$	76.60 (11)
$Mo1^{xvii}—Sr1—Sr1^{iv}$	61.57	$O1^{xii}—Sr1—O1^{xiii}$	134.61 (10)
$Mo1^{xvii}—Sr1—O1$	99.85 (8)	$O1^{xii}—Sr1—O1^{xiv}$	73.95 (11)
$Mo1^{xvii}—Sr1—O1^{x}$	80.15 (8)	$O1^{xii}—Sr1—O1^{xv}$	151.21 (11)
$Mo1^{xvii}—Sr1—O1^{ix}$	81.67 (8)	$O1^{xiii}—Sr1—O1^{xiv}$	151.21 (11)
$Mo1^{xvii}—Sr1—O1^{xi}$	98.33 (8)	$O1^{xiii}—Sr1—O1^{xv}$	73.95 (11)
$Mo1^{xvii}—Sr1—O1^{xii}$	24.34 (7)	$O1^{xiv}—Sr1—O1^{xv}$	77.98 (11)
$Mo1^{xvii}—Sr1—O1^{xiii}$	155.66 (7)	$Mo1—O1—Sr1$	133.45 (18)
$Mo1^{xvii}—Sr1—O1^{xiv}$	52.73 (8)	$Mo1—O1—Sr1^{iv}$	119.96 (15)
$Mo1^{xvii}—Sr1—O1^{xv}$	127.27 (8)	$Sr1—O1—Sr1^{iv}$	103.40 (13)
$Ca1—Sr1—Ca1^{viii}$	0		

Symmetry codes: (i) $-y+1/2, x-1, z-1/4$; (ii) $-y+1/2, x, z-1/4$; (iii) $-y+3/2, x-1, z-1/4$; (iv) $-y+3/2, x, z-1/4$; (v) $-x+1, -y+1, z$; (vi) $y, -x+1, -z$; (vii) $-y+1, x, -z$; (viii) $-y+1, x-1/2, z+1/4$; (ix) $-y+2, x-1/2, z+1/4$; (x) $-x+2, -y+1, z$; (xi) $y, -x+3/2, z+1/4$; (xii) $-x+2, -y+3/2, -z+1/4$; (xiii) $x, y-1/2, -z+1/4$; (xiv) $y+1/2, -x+3/2, -z+1/2$; (xv) $-y+3/2, x-1/2, -z+1/2$; (xvi) $-y+1, x+1/2, z+1/4$; (xvii) $-y+2, x+1/2, z+1/4$.