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Synthesis and crystal structure of a new strontium nitridomolybdate oxide, $Sr_4[MoN_4]O$

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The new ternary nitride oxide $Sr_4[MoN_4]O$ was synthesised by the reaction of strontium nitride with molybdenum nitride under a low partial pressure of oxygen in a sealed stainless steel crucible. Structure determination from single crystal X-ray data showed the structure to be monoclinic in the space group $P2_1/m$ (no. 11). The crystal morphology and strontium/molybdenum ratios were investigated using scanning electron microscopy and energy dispersive analysis by X-rays. The structure contains isolated $[MoN_4]^{6-}$ tetrahedra. Oxygen is ordered in the anion sublattice and is found only in the co-ordination sphere of the alkaline earth metal.

Introduction

Ternary and higher nitride research has grown steadily in importance over the last decade.[1–3] However, the nitrides remain little studied compared not only to oxides but also to other solid-state compounds such as halides and sulfides. Nitrides are observed to share some of the characteristics of both ionic and covalent compounds, principally as a consequence of the size and electronegativity of nitrogen. The interplay of these aspects often leads to new and unusual structures, yet it is the thermodynamics of the nitride anion (*versus* the oxide anion, for example) that often dictates ternary nitride formation.

With the growing number of these materials emerging, it is often useful to consider nitrides by structure type[1] or by co-ordination geometry of metals (or non-metals) to nitrogen.[2,3] Despite the rarity of nitrides compared to other solid state compounds, the number of ternary and higher compounds containing tetrahedrally co-ordinated metals or non-metals is relatively large. The first examples of tetrahedrally co-ordinated transition metals were reported several decades ago by Juza *et al.* in lithium–early transition metal nitrides.[4] Here, the *anti*fluorite superstructures contained discrete Li–N and M–N tetrahedral units ordered or disordered within the unit cell. Ternary nitrides formed with p-block elements are now becoming more widespread and tetrahedral co-ordination to nitrogen is the norm in these compounds. Linking of these tetrahedral units leads to an array of extended structures and recent advances in nitrido-silicate and -phosphate chemistry have illustrated a diversity in crystal chemistry potentially rivalling oxo systems.[5]

Among transition metal compounds, however, ternary and higher nitrides containing the heavier metals of Groups 5 and 6 appear to show the greatest tendency to form structures containing metals tetrahedrally co-ordinated to nitrogen.[2,6] Those containing molybdenum and tungsten are particularly numerous. Examples of structures exist in which tetrahedra are isolated or linked by one or more vertex, thus forming dimers and oligomers, one dimensional (1D) infinite chains of varying configuration, 2D sheets or 3D frameworks. The crystal chemistry of the nitridomolybdates and nitridotungstates has drawn comparison with silicates for obvious reasons.

One interesting aspect of many of these A–M–N systems (A = alkali and/or alkaline earth metals) is their ability to incorporate various mole fractions of oxygen into the anion sublattice without disrupting the transition metal–nitrogen bonding framework. Synthetically, this is unusual in ternary transition metal systems where attempts to partially oxidise nitrides usually result in formation of more thermodynamically stable oxide species. Here, we report the synthesis and subsequent characterisation of a new strontium molybdenum nitride oxide $Sr_4[MoN_4]O$. The oxynitride synthesis offers an example of how nitrides can be preferentially part oxidised in ternary Group 6 metal systems using a relatively low partial pressure of oxygen. The structure of the alkaline earth compound contains isolated $[MoN_4]^{6-}$ units and an ordered oxygen sublattice arrangement. After completion of this work, we were made aware of the existence of a report of $Sr_4[MoN_4]O$ unpublished in the open literature.[7] Comparisons to this report of the compound are drawn in our discussion.

Experimental

Starting materials

All manipulations were carried out in a nitrogen- or argon-filled glove box. Strontium nitride (Sr_2N) was prepared by reacting strontium metal dissolved in liquid sodium with nitrogen at 973 K. Strontium pieces (1–2 g) (Aldrich 99%) were cleaned of surface oxide in an evacuable argon-filled glovebox (*ca.* 5 ppm O_2, <5 ppm water). The pieces were dissolved in an excess of liquid sodium at 250 °C, contained in a stainless steel crucible. On cooling, the crucible was sealed inside a stainless steel vessel which was then removed from the box, connected to a vacuum/gas line and evacuated. The vessel was heated under a positive nitrogen pressure (*ca.* 2 atm) at 973 K for 48 h as described more fully elsewhere.[8] The excess sodium was removed from the product by vacuum distillation at 623 K for 24 h. Liquid sodium is unreactive towards nitrogen and serves as an inert solvent for the alkaline earth metals. This method was found to produce nitrides containing negligible amounts of alkaline earth oxide. The reaction yielded polycrystalline samples of purple–black strontium nitride. The identity of the nitride was confirmed by powder X-ray diffraction (PXD) using a Philips XPERT θ–2θ diffractometer (Cu-Kα radiation) with reference to the ICDD (JCPDS) database.

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Synthesis of $Sr_4[MoN_4]O$

Single crystals of $Sr_4[MoN_4]O$ were prepared by the solid state reaction of the binary alkaline earth nitride Sr_2N with nominally Mo_2N powder (Goodfellows 99.5%). The reactivity of the alkaline earth nitride towards water and oxygen necessitated that all manipulations were carried out in an argon-filled glove box. The purity of the binary molybdenum nitride was assessed by powder X-ray diffraction. Subsequent phase identification and Rietveld refinement of the pattern (using the Philips PC RIETVELD PLUS package)[9,10] showed that, in fact, it was composed of a mixture of Mo_2N (77.3 wt%) and Mo (22.7 wt%). The reagents were mixed in a 7.92 : 1 molar ratio, based on an average reactant composition of 2.23 : 1 Mo : N. The reactants were thoroughly ground and pressed together into a pellet using a hand press. The pellet was then wrapped in molybdenum foil and placed in a stainless steel crucible, which was subsequently welded closed under an argon atmosphere. The crucible was heated to 1393 K for 5 days under a constant stream of argon (to prevent oxidation of the steel crucible) and then slowly cooled to room temperature at 20 K h^{-1}. Visual examination of the outside of the steel crucible after reaction revealed that the welds had experienced severe strain during the course of the reaction and that some oxygen may have been admitted to the system *via* a small 'pinhole' leak. The cooled crucible was mechanically cleaned and opened in a nitrogen-filled glovebox. The product was observed as a mass of dark blue crystals contained within the molybdenum tube. Further crystals of a similar colour and habit were also observed on the surface of the molybdenum foil surrounding the bulk product. Single crystals were obtained as fragments of the bulk product.

Structure determination

The crystals obtained were loaded into 0.2 mm diameter glass capillaries (which had been previously degassed by heating at 573 K for 24 h at *ca.* 10^{-5} Torr) in a nitrogen filled glovebox. The crystal quality was assessed by taking Weissenberg photographs. The crystal used for structure determination was removed from the capillary by breaking it under RS3000 oil. The crystal was then further cut to reduce absorption effects to final dimensions of 0.35 × 0.31 × 0.13 mm. Single crystal X-ray diffraction data were collected on a Stoe Stadi 4 four-circle diffractometer using graphite monochromated Mo-Kα radiation. The structure was solved using the direct methods software, SIR97.[11] Two trial stoichiometries were tested, Sr_3MoN_4 and Sr_6MoN_6 both giving solutions with $R \approx 0.09$ for similar numbers of atoms. The electronic configurations of Sr^{2+} and Mo^{6+} are identical and hence had to be assigned on the basis of their bond lengths to nitrogen. The trial structure, comprising 3 Mo, 10 Sr and 13 N atoms was then refined using SHELXL-97.[12] As the refinement progressed it became apparent that this corresponded to a stoichiometry of 'Sr_4MoN_5', which implies an impossible oxidation state of 7+ for molybdenum. Close inspection of the bond length data revealed that three of the N atoms were not bonded to any molybdenum atoms. Reassigning these atoms as oxygen gave the final stoichiometry Sr_4MoN_4O and refinement proceeded smoothly to a final *R* of 0.048 [$I > 2\sigma(I)$]. The crystallographic parameters are summarised in Table 1.

CCDC reference number 186/1827.

See http://www.rsc.org/suppdata/dt/a9/a907843f/ for crystallographic files in .cif format.

Table 1 Diffraction data for Sr_4MoN_4O

Empirical formula	Sr_4MoN_4O
M	518.46
T/K	293(2)
λ/Å	0.71073
Crystal system	Monoclinic
Space group	$P2_1/m$
Unit cell dimensions	
a/Å	8.951(11)
b/Å	14.694(12)
c/Å	10.715(10)
β/°	102.08(7)
V/Å^3	1378(2)
Z	8
μ/mm^{-1}	32.457
Reflections collected/unique (R_{int})	3575/2532 (0.0665)
Final *R* indices [$I > 2\sigma(I)$]	$R1^a = 0.0480$, $wR2^b = 0.1175$
R indices (all data)	$R1^a = 0.0671$, $wR2^b = 0.1303$
Largest diff. peak and hole/e Å^{-3}	2.330 and −1.847

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma w(|F_o^2| - |F_c^2|)^2/\Sigma w(F_o^2)^2]^{\frac{1}{2}}$, $w = \sigma(F_o)^{-2}$.

Bulk structure and analysis

To confirm the structure as being representative of the bulk phase powder X-ray diffraction data were collected for *ca.* 150 mg of the crystalline sample using a Philips XPERT θ–2θ diffractometer with Cu-Kα radiation. Samples for PXD were loaded in a nitrogen-filled recirculating glovebox (*ca.* 1 ppm O_2, <5 ppm water) into specially designed sample holders for measuring diffraction data from air-sensitive samples. Scans were run over *ca.* 1–3 h over a 2θ range 5–120° with step size of 0.02° in 2θ. Calculated PXD patterns were generated from the final single crystal diffraction data using the PC software package POWDERCELL 2.0.[13] The observed patterns matched well with the calculated pattern for $Sr_4[MoN_4]O$ (Fig. 1) but some extra weaker lines are also observed. These lines could not be identified and the relative intensities were observed to change relative to the major $Sr_4[MoN_4]O$ phase over different PXD experiments. This would suggest that at least one further (possibly ternary) phase is present in the bulk sample, albeit as a minor component in the reaction products.

The morphology of the crystalline products was evaluated by scanning electron microscopy (SEM) using a Phillips XL 30 ESEM-FEG instrument running at either 10.0 or 15.0 kV in ultra high vacuum mode. Simultaneous energy dispersive analysis by X-rays (EDAX) was performed to determine the Sr : Mo ratio. Samples were loaded into the SEM under a stream of nitrogen gas to minimise reaction with air. Micrographs of the crystalline fragments show particles of irregular blocky habit of approximate dimensions 500 × 300 μm. Taking spot scans over several different crystallites, values of 80.90(1) atom% Sr and 19.09(1) atom% Mo were recorded, yielding a Sr : Mo ratio of 4.2 : 1, in good agreement with the crystallographically determined stoichiometry.

Results and discussion

$Sr_4[MoN_4]O$ crystallises in monoclinic space group $P2_1/m$. Our refined structural model is in agreement to that reported by Höhn.[7] The structure of the oxynitride is complex and is made up of densely packed, highly distorted, edge-sharing Sr–(N,O) polyhedra with coordination numbers six and seven. Isolated MoN_4 tetrahedra exist inserted in the cavities within this Sr-centred polyhedral network; hence Mo^{6+} ions are located in tetrahedral holes bounded *only* by nitrogen (Fig. 2).

Depictions of structures in terms of nitrogen-centred polyhedra are often useful in ternary nitride systems, where the coordination number of nitrogen is often higher than that of the constituent cations. However, in $Sr_4[MoN_4]O$ the nitrogen-centred polyhedra (which are highly distorted and are of coordination number five and six) edge-share to form an elaborate three dimensional array and in this case, the N-centred polyhedral approach does not present a particularly informative representation of the structure. Clearer interpretations of the structure can be obtained by considering the arrangement of the Mo–N tetrahedra and the oxygen centred polyhedra either in isolation or in combination.

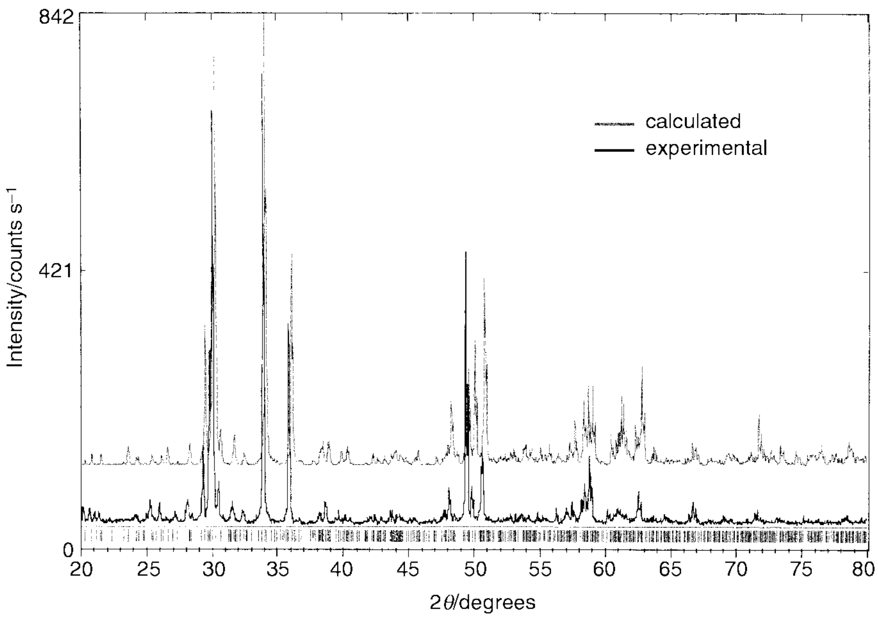

Fig. 1 Observed (black; lower profile) and calculated (grey; upper profile) powder diffraction patterns of $Sr_4[MoN_4]O$. The calculated pattern is derived from the single crystal data.

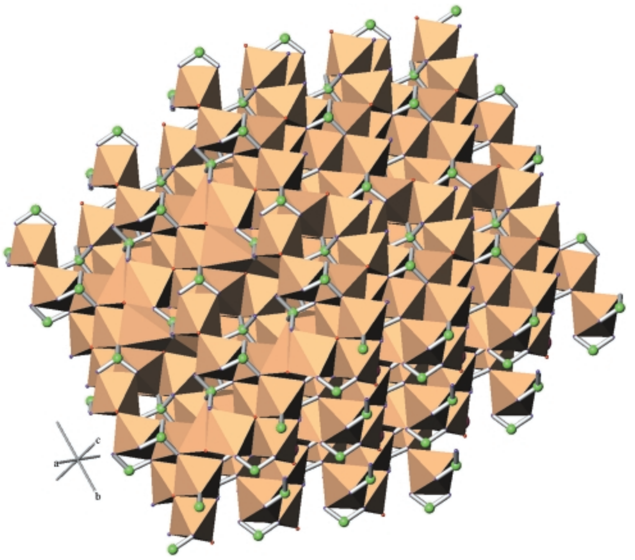

Fig. 2 Structure of $Sr_4[MoN_4]O$ as a projection on the [111] plane, showing the isolated MoN_4 tetrahedra (ball and stick representation) within the cavities of the Sr–(N,O) framework (polyhedra).

The discrete Mo–N tetrahedra align in rows (or unlinked 'layers') of varying orientation which are apparent when viewed along any of the three crystallographic directions. Perhaps the simplest of these views of the Mo–N sublattice, however, is seen as projection on the [010] plane [Fig. 3(a)]. In this view, rows of $[MoN_4]^{6-}$ anions run parallel to the *a* and *c* axes. Considering the rows parallel to the *c*-direction, there are four row types arranged ..ABCDA.. along *a*. Row B contains tetrahedra oriented in the opposite direction to row A and row D likewise with row C. The same pattern exists in the rows *parallel* to the *a*-direction (..A′B′C′D′A′…). It should be remembered, however, that these rows do not lie within a flat plane and the view in the [001] plane illustrates the displacement of the tetrahedra along the *b*-direction [Fig. 3(b)]. In this view, successive 'layers' of tetrahedra [marked I, II, III and IV in Fig. 3(b)] can be regarded as stacking along the *b* axis (at $y = 0.25$, 0.48, 0.75, 0.98).

Considering now the arrangement of oxygen-centred polyhedra, each oxygen ion sits at the centre of an octahedron with strontium ions at each vertex. These octahedra link by vertices

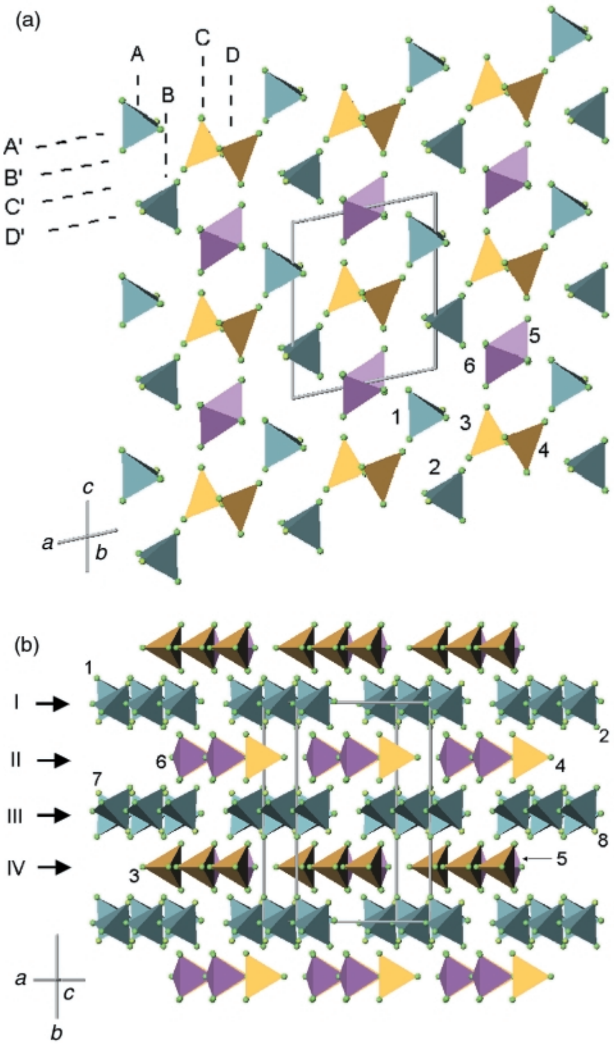

Fig. 3 Polyhedral representations of the $Sr_4[MoN_4]O$ crystal structure illustrating the arrangement of isolated MoN_4 tetrahedra, (a) as a projection on the [010] plane (b) as a projection on the [001] plane. Each different tetrahedron orientation is marked 1–8 for clarity, but note orientations 7 and 8 are obscured by 1 and 2 in (a). Distinct rows are marked A,B,C,D and A′B′C′D′ in (a) and distinct "layers" I, II, III, IV in (b).

Table 2 Selected bond lengths and angles

Atoms	Distance/Å	Bond angles/°	Atoms	Distance/Å	Bond angles/°
Mo1 N2	1.86(3)	105.5(4)–124.4(7)	Mo2 N5	1.82(2)	103.9(5)–115.0(5)
N8	1.88(4)		N3	1.87(2)	
N7	1.91(2) × 2		N4	1.89(2)	
			N6	1.91(2)	
Mo3 N1	1.87(3)	104.8(9)–114.7(6)			
N10	1.84(4)				
N9	1.84(3) × 2				
Sr1 O2	2.39(3)	61.9(6)–175.5(5)	Sr2 O2	2.37(3)	60.9(3)–175.1(5)
O3	2.53(3)		N10	2.40(4)	
N3	2.70(2) × 2		N6	2.67(2) × 2	
N9	2.84(3) × 2		N8	3.22(3)	
			N5	3.23(3) × 2	
Sr3 N9	2.52(2)	65.6(4)–178.7(3)	Sr4 N9	2.56(3)	67.6(5)–161.1(3)
O1	2.61(2)		O2	2.72(2)	
O3	2.64(2)		N1	2.79(2)	
N4	2.65(2)		N6	2.81(2)	
N7	2.67(2)		N5	2.82(3)	
N2	2.88(3)		O1	2.86(2)	
Sr5 N1	2.56(3)	73.2(5)–176.4(5)	Sr6 O1	2.43(2)	66.8(3)–176.1(3)
O3	2.60(3)		N6	2.66(2)	
N7	2.61(2) × 2		N3	2.74(2)	
N6	2.66(2) × 2		N7	2.77(2)	
			N4	2.85(2)	
			N7′	2.95(2)	
Sr7 O1	2.50(2) × 2	72.2(4)–180.00(1)	Sr8 O3	2.50(2)	70.9(4)–169.9(4)
N9	2.62(3) × 2		N6	2.62(2)	
N5	2.83(2) × 2		N4	2.66(2)	
			N8	2.66(3)	
			N3	2.67(2)	
			N4′	2.78(2)	
Sr9 O1	2.52(2)	61.7(3)–178.7(3)	Sr10 N5	2.52(2)	74.5(5)–167.3(3)
N7	2.61(2)		N2	2.57(2)	
N4	2.69(2)		O1	2.60(2)	
N8	2.77(2)		N3	2.61(2)	
N1	2.85(2)		O2	2.62(2)	
N10	3.01(4)		N10	2.81(4)	
N5	3.24(3)				

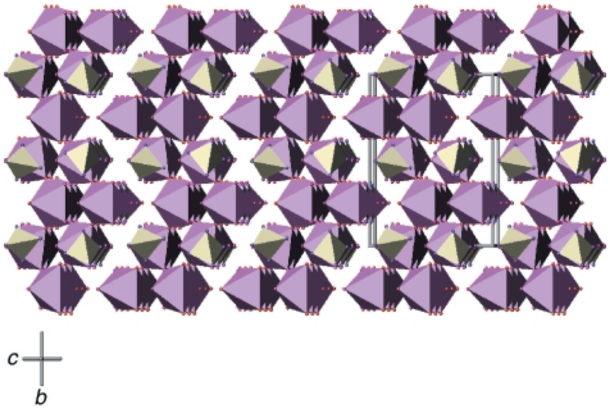

Fig. 4 Structure of $Sr_4[MoN_4]O$ as a projection on the [100] plane, showing double layers of vertex-sharing OSr_6 octahedra (purple) and superimposed isolated MoN_4 tetrahedra (yellow).

to form buckled double-layers stacked along the crystallographic *b*-direction (Fig. 4). The Mo–N tetrahedra are located within, rather than between, these double layers when viewed as a projection on the [100] plane.

Important interatomic distances and angles are listed in Table 2. These distances and angles are generally in good agreement with those reported by Höhn.[7] The MoN_4 units themselves, in $Sr_4[MoN_4]O$, are distorted slightly from the ideal tetrahedral geometry. Bond lengths vary between 1.82(2) and 1.91(2) Å while the bond angles observed range from 103.9(5) to 124.4(7)°. Höhn observes comparable tetrahedral distortion in his refinement of the structure and reports very similar ranges of distances and angles [Mo–N 1.81(3)–1.91(2) Å and N–Mo–N 105.36(1)–124.00(1)°].[7] This distortion is larger than in other nitridometalates where bond angles are typically between 106 and 112°. In those Group 6 oxonitridometalates previously reported, however, tetrahedral distortions follow a similar pattern to $Sr_4[MoN_4]O$ with observed angles also in the range 105–126°.[2a,6] The mean bond length [1.87(2) Å] agrees well with those in other A–Mo–(N,O) compounds containing isolated Mo–N tetrahedra {*e.g.* Li_6MoN_4, 1.879 Å; Ba_3MoN_4, 1.87 Å; $Li_6Ca_{12}[MoN_4]_4O_3$, 1.88 Å}.[14–16]

The strontium coordination environment is more irregular. Strontium cations are six and seven coordinate to nitrogen and oxygen. The majority adopts a highly distorted octahedral geometry with either one or two oxygen atoms in the co-ordination sphere. Bond lengths vary between 2.93(3) Å (Sr1–O2) and 2.88(2) Å (Sr3–N2) within these octahedra. The seven coordinate strontium ions (Sr2, Sr9) contain only one oxygen ligand within the first coordination sphere and demonstrate a larger variation in bond length [*e.g.* Sr2 2.37(3)–3.23(3) Å] than those that are octahedrally co-ordinated. Notable distortions of the alkaline earth cation environment can also be observed in other nitridometalates. In Ba_3MoN_4, for example, the barium nitrogen distances vary between 2.71(1) and 3.56(1) Å.[15]

Bond valence calculations were performed, using appropriate parameters for the metals with nitride and oxide ions, for each

Table 3 Bond valence sums for Sr and Mo sites in $[Sr_4MoN_4]O$

Site	Valence
Sr1	1.8
Sr2	1.9
Sr3	1.8
Sr4	1.4
Sr5	2.0
Sr6	1.6
Sr7	1.8
Sr8	1.9
Sr9	1.6
Sr10	1.9
Sr_{mean}	1.8
Mo1	6.0
Mo2	6.3
Mo3	6.7
Mo_{mean}	6.3

of the cation and anion sites in $Sr_4[MoN_4]O$.[17] The results are shown in Table 3 (valence sums for the anion sites have been omitted for brevity). The calculated valence sums for Sr give a mean of 1.8; slightly less than the expected value, as is often observed in nitrides. Two of the three Mo ions have valence sums exceeding their expected (and maximum) oxidation state. The absolute, quantitative values from bond valence calculations for transition metals in nitrides are frequently higher than expected. The calculated values for Mo in $Sr_4[MoN_4]O$ are no exception. However, importantly, the implication is that there is significant π-character in the Mo–N bonding framework. Calculations performed from published data for the nitridomolybdates Li_6MoN_4 and Ba_3MoN_4,[15,16] both containing isolated Mo–N tetrahedra, yield very similar values for the Mo valence (6.2 and 6.4, respectively). Hence, despite the presence of highly electropositive counter cations, Mo–N bonding is significantly covalent. This behaviour is also observed in nitrides containing *linked* $Mo(W)N_4$ tetrahedra. In these 1D compounds, it is often the terminal Mo(W)–N bonds that show the greatest π-character, although as the tetrahedral connectivity increases, the degree of π-character in the bonds to the bridging ligands also increases.[6]

In ternary oxide compounds, molybdenum and tungsten commonly coordinate to oxygen in octahedral geometries [*e.g.* $Mo(W)O_3$, polymolybdates and polytungstates, *etc*.]. Oxides containing the tetrahedral $[Mo(W)O_4]^{2-}$ anion, for example, are well known but less numerous.[18] In molybdenum and tungsten ternary *nitrides* (where the total metal : anion ration is usually higher by virtue of the increased anionic charge, reduced oxidation number, of N^{3-} over O^{2-}) coordination numbers higher than four are exceptional [an example of an exception is $LiMo(W)N_2$,[19] containing nominally Mo (or W) (V)]. The majority of nitrido-molybdates and -tungstates contain transition metals in tetrahedral coordination. Isolated MN_4 tetrahedra are observed in compounds containing electropositive cations {*e.g.* Li_6MN_4,[14] $Ba_3[MN_4]$ (M = Mo, W)[15] and $Ca_2Sr[WN_4]$[20]} and link by vertices to form dimers in, for example, $LiBa_4[M_2N_7]$ (M = Mo, W).[21] Nitrides containing sodium and the heavier alkali metals form more condensed structures with Mo(W)–N tetrahedra linking at vertices to create infinite chains (*e.g.* $Na_3[MN_3]$ (M = Mo, W), $Na_5Rb(Cs)(WN_3)_2$, $Na_2K[WN_3]$, $Na_{11}Rb[(WN_3)_4]$).[22–24]

Within known *oxy*nitrides of molybdenum and tungsten, one might expect, therefore, the transition metal coordination to reflect the degree of oxide or nitride 'character' and the oxygen : nitrogen ratio. However, in most cases, oxynitrides have a crystal chemistry broadly similar to nitridometalates. There are a few examples of oxygen-rich oxonitrido-molybdates and -tungstates containing octahedral Mo or W (*e.g.* $SrMoO_{2.5}N_{0.5}$, $SrWO_2N$, both with the perovskite structure).[25] Nitrogen-rich ternary oxynitrides contain tetrahedral Mo(W)–N species without exception. Yet, there are also examples of compounds with high O : N ratios also containing only tetrahedral Mo or W {*e.g.* $Ba_3[WNO_3]_2$, $Na_3[Mo(W)NO_3]$}.[26,27]

Hence, isolated and linked tetrahedra are observed in the vast majority of ternary (and higher) molybdenum and tungsten oxynitrides. The distribution of oxygen and nitrogen within the anionic sublattice appears to be dependent on the electropositivity and also, perhaps, the size of the s-block countercation. In, for example, the alkali metal compounds $Na_3[MNO_3]$, $Na_4[MN_2O_2]$ and $A_6[M_2N_4O_3]$ (A = Na, K, Rb, Cs; M = Mo, W), oxygen and nitrogen are apparently randomly distributed over the anion sites.[27–29] In $Ca_{51}[WN_4]_{12}N_8O_3$, $Sr_{51}[WN_4]_{12}N_8O_3$, $Li_6Ca_{12}[MN_4]_4O_3$, however, the oxygen and nitrogen positions are distinct.[16,30] Within these anion ordered structures, the oxygen ions coordinate exclusively to the alkali and/or alkaline earth metals leaving the Group 6 metal only bonded to nitrogen. This behaviour is further evident in $Sr_4[MoN_4]O$ where there are no molybdenum–oxygen bonds. Previously, this preference has been proposed to be thermodynamically driven by the high stability of lithium and calcium oxides, for example, compared to their nitrides.[16] This relative stability should likewise apply to the heavier alkaline earth metals in oxonitridometalates. Given that a similar ordering of oxygen around the alkaline earth cation occurs in the oxynitride $Ba_3[ZnN_2]O$,[31] the stability of the A^{II}–O bond may well be the driving force in determining the anion distribution in $Sr_4[MoN_4]O$. Lithium is the only alkali metal to form a stable binary nitride. Why the heavier alkali metal oxonitridometalates should not seemingly exhibit a similar oxygen distribution on this basis is perhaps, therefore, an intriguing question.

In summary we have synthesised the new ternary molybdenum nitride oxide $Sr_4[MoN_4]O$. The partial oxidation to yield this compound is possible *via* reaction with a low partial pressure of oxygen. In similarity to other known examples of nitrides and oxynitrides of molybdenum and tungsten, the transition metal is co-ordinated to nitrogen in isolated tetrahedra. Oxygen bonds exclusively to the alkaline earth cation, Sr^{2+}.

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