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Supplementary material

Can we predict the formability of perovskite oxynitrides from tolerance and octahedral factors?

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Structure field map

Table S 1. Tolerance and octahedral factors of perovskite oxynitrides synthesized so far. The tolerance and octahedral factors are calculated according to the eqs. 1 and 2 and Table 3 (see main text).

Material/Ref	Structure	Parameters calculated from interatomic distance[a]		Ref	Parameters calculated from ionic radii for oxides[b]	
		Tolerance factor	Octahedral factor		Tolerance factor	Octahedral factor
$SrWO_2N$	*Pm*-3*m*	0.9998	0.3891	[1]	0.989616	0.432789
$SrMoO_{2.5}N_{0.5}$	*Pm*-3*m*	0.9996	0.3884	[2]	0.994462	0.425808
$BaTaO_2N$	*Pm*-3*m*	1.0420	0.4354	[3]	1.038066	0.446750
$BaNbO_2N$	*Pm*-3*m*	1.0420	0.4409	[4]	1.038066	0.446750
$EuNbO_2N$	*Pm*-3*m*	0.9870	0.4073	[5]	0.979383	0.44674963
$EuTaO_2N$	*Pm*-3*m*	0.9991	0.4031	[6]	0.979383	0.44674963
$EuWO_{1.58}N_{1.42}$	*Pm*-3*m*	0.9998	0.3718	[7]	0.988927	0.4327887
$LaNbON_2$	*Pnma*	0.9842	0.4054	[8]	0.948883	0.436593
$CaTaO_2N$	*Pnma*	0.9490	0.4161	[9]	0.945947	0.446750
	Pnma	0.9808	0.4100	[6]		
$NdTiO_2N$	*Pnma*	0.9410	0.3955	[10]	0.937905	0.422318
$LaZrO_2N$	*Pnma*	0.9200	0.4903	[9]	0.917357	0.502593
$SrNbO_2N$	*Pnma*	0.9969	0.4155	[11]	0.980065	0.446750
$PrZrO_2N$	*Pmna*	0.8618	0.5008	[2]	0.921956	0.502593
$NdZrO_2N$	*Pmna*	0.8625	0.4938	[12]	0.887791	0.502593
$SmZrO_2N$	*Pmna*	0.8272	0.5217	[12]	0.877936	0.50259333
$CaMoO_{1.7}N_{1.3}$	*Pbnm*	0.9823	0.3921	[13]	0.959842	0.425808
$NdVO_2N$[*1]	*Pbnm*	0.9745	0.3486	[14]	0.949557	0.40486685
$CaNbO_2N$	*I*4/*mcm*	0.9191	0.4203	[15]	0.945947	0.446750
$SrTaO_2N$	*I*4/*mcm*	0.9986	0.4098	[16]	0.980065	0.446750
		0.9982	0.4085	[17]		
		0.9973	0.4105	[9]		
$LaWO_{0.6}N_{2.4}$	*I*-4	1.0046	0.3593	[18]	0.957983	0.422949
$LaTiO_2N$	*Imma*	0.9860	0.3974	[10]	0.969139	0.422318
$LaTaON_2$	*C*2/*m*	0.9560	0.3982	[16]	0.948883	0.436593
$LaVO_{2.1}N_{0.9}$[*2]	-	-	-	[19]	0.981180	0.404867
$NdWO_{0.8}N_{2.2}$[*2]	-	-	-	[20]	0.927472	0.42294916
$NdNbON_2$[*2]	*Pnma*	-	-	[21]	0.918663	0.43659269
$PrNbON_2$[*2]	*Pnma*	-	-	[21]	0.953584	0.436593

[*1]: structure refinement is performed; the cation-anion distances $d_{A\text{-}X}$ is not available

[*2]: structure refinement is not performed; the cation-anion distances $d_{A\text{-}X}$ and $d_{B\text{-}X}$ are not avilable

[a]: caculated based on average cation-anion distances from refinement results of neutron diffraction (see main text Table 5 and 8)

[b]: caculated based on ionic radii for oxides (see main text Table 6 and 8)

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Table S 2. Tolerance and octahedral factors of non-perovskite oxynitrides. The tolerance and octahedral factors are calculated according to the eqs. 1 and 2 and Table 3(see main text).

Material/Ref	Structure Space Group	Parameters under room temperature		Ref
		Tolerance factor	Octahedral factor	
$Mn_2(MnTa_3)N_{6-x}O_{2+x}$	Spinel *Fd3m*	0.7015	0.4728	22
$NdWO_{3.05}N_{0.95}$	Scheelite *I*41*/a*	0.9679	0.2621	7
$KOsO_3N$	Scheelite *I*41*/a*	1.1641	0.2020	23
$RbOsO_3N$	Scheelite *I*41*/a*	1.7936	0.1921	24
Sr_2TaO_3N	K_2NiF_4 *I4/mmm*	0.7489	0.4090	25, 26
Ba_2TaO_3N	K_2NiF_4 *I4/mmm*	0.7598	0.4272	13, 27
$Sr_2NbO_{2.8}N$	K_2NiF_4 *I4/mmm*	0.7484	0.4112	28
$Nb_{0.6}Al_{0.08}O_{0.21}N_{0.79}$	Rock-salt *I4/m*	0.7581	0.4020	29
$Nd_2Ta_2O_5N_2$	Pyrochlore	0.7757	0.4380	30
Na_3WO_3N	Others *Pmn*21	0.8457	0.0332	31
Na_3MoO_3N	Others *Pmn*21	0.8404	0.0379	32
Ba_3ZnN_2O	Others *P4/mmm*	0.9897	0.2709	33
$Ba_3W_2O_{6.27}N_{1.73}$	Others *R*-3*m*	3.6632	0.0325	34
$Ba_3Mo_2O_{6.04}N_{1.96}$	Others *R*-3*m*	3.6589	0.0255	32
Ba_2VO_3N	Others *Pnma*	1.0354	0.2076	25

Table S 3 The bond distance A-X, B-X, tolerance and octahedral factors based on geometric and arithmetic means

Composition			$LaNbON_2$	$CaTaO_2N$	$SrTaO_2N$	$LaTiO_2N$	$CaMoO_{1.7}N_{1.3}$	$LaWO_{0.6}N_{2.4}$	$CaNbO_2N$	$SrNbO_2N$	$NdVO_2N$
Experimental data by Neutron diffraction	Geometric mean	A-X	2.8677	2.802	2.8523	2.7915	2.7707	2.8311	2.6446	2.8591	2.7245
		B-X	2.0602	2.02	2.0197	2.002	1.9943	1.9927	2.0346	2.0278	1.9769
		t	0.9842	0.9809	0.9986	0.986	0.9824	1.0046	0.9191	0.9970	0.9745
		O_t	0.4054	0.4100	0.4098	0.3974	0.3921	0.3593	0.4203	0.4155	0.3486
	Arithmetic mean	A-X	2.8798	2.8167	2.8533	2.7991	2.7862	2.834	2.6556	2.8615	2.7373
		B-X	2.0602	2.02	2.0197	2.002	1.9943	1.9927	2.0347	2.0278	1.977
		t	0.9886	0.9861	0.9991	0.9888	0.9880	1.0058	0.9230	0.9980	0.9792
		O_t	0.4054	0.4100	0.4098	0.3975	0.3921	0.3594	0.4203	0.4154	0.3800
Prediction by ionic radii	Geometric mean	A-X	2.8263	2.7729	2.8729	2.7929	2.7729	2.8263	2.7729	2.8729	2.7029
		B-X	2.1061	2.0728	2.0728	2.0378	2.0428	2.0861	2.0728	2.0728	2.0128
	Arithmetic mean	A-X	2.8267	2.7733	2.8733	2.7933	2.7733	2.8267	2.7733	2.8733	2.7033
		B-X	2.1067	2.0733	2.0733	2.0383	2.0433	2.0867	2.0733	2.0733	2.0133

t: tolerance factor; O_t: Octahedral factor

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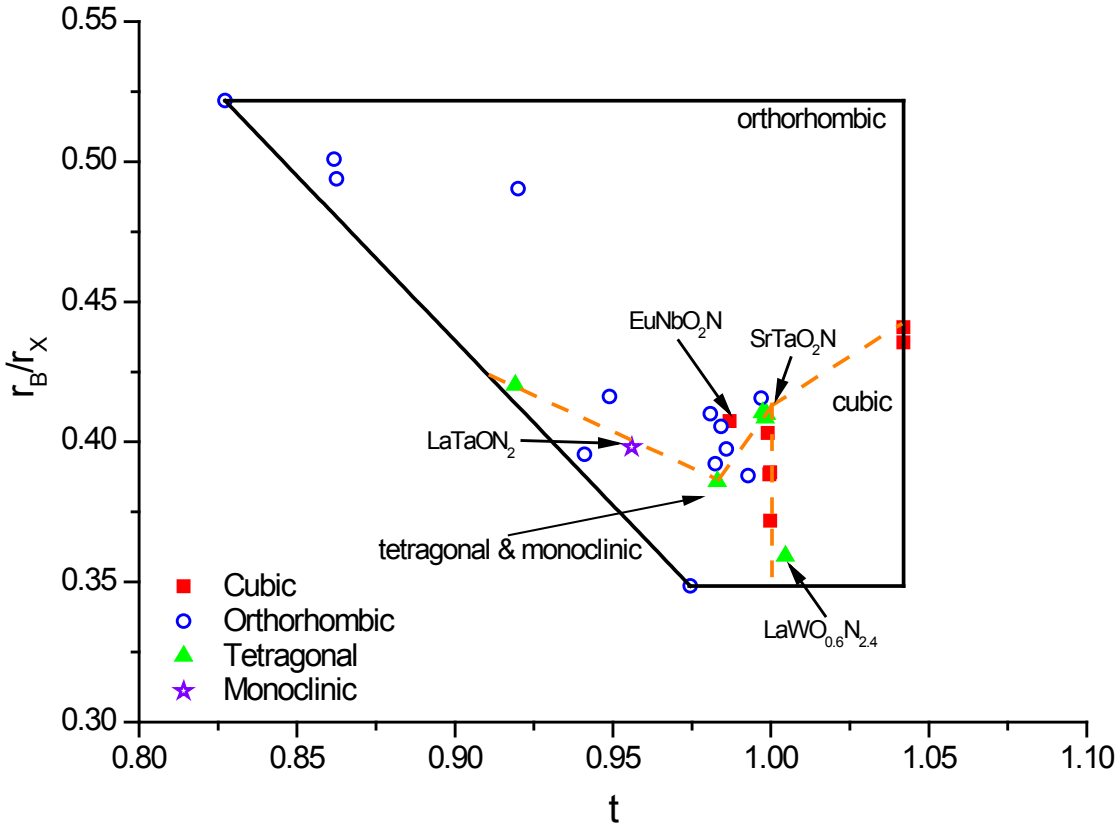
Figure S1. Location of perovskite oxynitrides with different crystal symmetry in the structure field map from Figure 2.



Prediction

Table S 4. Combination of A and B cations in $AB(O,N)_3$ perovskites applied for the calculation of the tolernace and ocathaderal factors listed in the Table S4 and displayed in the Figure 3.

$AB(O,N)_3$ perovskites	**A-site**	**B-site**
$A^{+}B^{6+}O_2N$	Li^{+}, Na^{+}, K^{+}	Mo^{6+}, W^{6+}
$A^{2+}B^{5+}O_2N$	Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Zn^{2+}, Cd^{2+}, Eu^{2+}	V^{5+}, Nb^{5+}, Ta^{5+}, Mo^{5+}, W^{5+}
$A^{2+}B^{6+}ON_2$	Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Zn^{2+}, Cd^{2+}, Eu^{2+}	Mo^{6+}, W^{6+}
$A^{3+}B^{4+}O_2N$	Sc^{3+}, Y^{3+}, Ga^{3+}, In^{3+}, La^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}	Si^{4+}, Ge^{4+}, Sn^{4+}, Ti^{4+}, Zr^{4+}, Hf^{4+}, Mn^{4+}, Fe^{4+}, Co^{4+}, V^{4+}, Nb^{4+}, Ta^{4+}, Mo^{4+}, W^{4+}
$A^{3+}B^{5+}ON_2$	Sc^{3+}, Y^{3+}, Ga^{3+}, In^{3+}, La^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}	V^{5+}, Nb^{5+}, Ta^{5+}, Mo^{5+}, W^{5+}

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Table S 5. Tolerance and octahedral factors of metal oxynitrides calculated according to the Table 6 (see main text). These factors are applied in the Figure 3 (see main text). "S" refers for perovskite oxynitrides synthesized so far, "P" stays for the perovskite oxynitrides predicted in our model, N - for perovskite structure is not stable, non-stoichiometric perovskite

Compounds	t	r_B/r_X	Formability
ABO_2N A^+B^{6+}			
$LiMoO_2N$	0.938464	0.41184731	P
$LiWO_2N$	0.933846	0.41882777	P
$NaMoO_2N$	0.986816	0.41184731	P
$NaWO_2N$	0.98196	0.41882777	P
$KMoO_2N$	1.07422	0.41184731	N
KWO_2N	1.068934	0.41882777	N
$A^{2+}B^{5+}$			
$MgVO_2N$	0.940854	0.376945	N
$MgNbO_2N$	0.895451	0.44674963	N
$MgTaO_2N$	0.895451	0.44674963	N
$MgMoO_2N$	0.908605	0.42580824	N
$MgWO_2N$	0.904178	0.4327887	N
$CaVO_2N$	0.993910	0.376945	N
$CaNbO_2N$	0.945947	0.446750	S/P
$CaTaO_2N$	0.945947	0.446750	S/P
$CaMoO_2N$	0.959842	0.425808	S[a]/P
$CaWO_2N$	0.955165	0.432789	P
$SrVO_2N$	1.029758	0.376945	N
$SrNbO_2N$	0.980065	0.446750	S/P
$SrTaO_2N$	0.980065	0.446750	S/P
$SrMoO_2N$	0.994462	0.425808	S[a]/P
$SrWO_2N$	0.989616	0.432789	S/P
$BaVO_2N$	1.090699	0.376945	N
$BaNbO_2N$	1.038066	0.446750	S/P
$BaTaO_2N$	1.038066	0.446750	S/P
$BaMoO_2N$	1.053314	0.425808	N
$BaWO_2N$	1.048182	0.432789	N
$ZnVO_2N$	0.941693	0.376945	N
$ZnNbO_2N$	0.89625	0.44674963	N
$ZnTaO_2N$	0.89625	0.44674963	N
$ZnMoO_2N$	0.909415	0.42580824	N
$ZnWO_2N$	0.904984	0.4327887	N
$CdVO_2N$	0.983155	0.376945	N
$CdNbO_2N$	0.935711	0.44674963	P
$CdTaO_2N$	0.935711	0.44674963	P
$CdMoO_2N$	0.949457	0.42580824	P
$CdWO_2N$	0.94483	0.4327887	P
$EuVO_2N$	1.029041	0.376945	N
$EuNbO_2N$	0.979383	0.44674963	S/P
$EuTaO_2N$	0.979383	0.44674963	S/P
$EuMoO_2N$	0.99377	0.42580824	P
$EuWO_2N$	0.988927	0.4327887	S[a]/P
$A^{3+}B^{4+}$			
$ScSiO_2N$	0.973386	0.27921852	N
$ScGeO_2N$	0.908896	0.36996453	N
$ScSnO_2N$	0.840373	0.48165194	N
$ScTiO_2N$	0.875436	0.42231801	N
$ScZrO_2N$	0.82866	0.50259333	N
$ScHfO_2N$	0.832528	0.49561287	N
$ScMnO_2N$	0.908896	0.36996453	N
$ScFeO_2N$	0.884115	0.40835708	N
$ScCoO_2N$	0.908896	0.36996453	N
$ScVO_2N$	0.886312	0.40486685	N
$ScNbO_2N$	0.844352	0.47467148	N
$ScTaO_2N$	0.844352	0.47467148	N
$ScMoO_2N$	0.856517	0.45373009	N
$ScWO_2N$	0.852423	0.46071055	N
$YSiO_2N$	1.035629	0.27921852	N
$YGeO_2N$	0.967015	0.36996453	N
$YSnO_2N$	0.894111	0.48165194	P
$YTiO_2N$	0.931415	0.42231801	P
$YZrO_2N$	0.881648	0.50259333	P
$YHfO_2N$	0.885764	0.49561287	P
$YMnO_2N$	0.967015	0.36996453	N
$YFeO_2N$	0.94065	0.40835708	P
$YCoO_2N$	0.967015	0.36996453	N
YVO_2N	0.942987	0.40486685	P
$YNbO_2N$	0.898344	0.47467148	P
$YTaO_2N$	0.898344	0.47467148	P
$YMoO_2N$	0.911286	0.45373009	P
YWO_2N	0.906931	0.46071055	P
$GaSiO_2N$	0.966324	0.27921852	N
$GaGeO_2N$	0.902302	0.36996453	N
$GaSnO_2N$	0.834277	0.48165194	N
$GaTiO_2N$	0.869074	0.42231801	N
$GaZrO_2N$	0.822638	0.50259333	N
$GaHfO_2N$	0.826488	0.49561287	N
$GaMnO_2N$	0.902291	0.36996453	N
$GaFeO_2N$	0.87769	0.40835708	N
$GaCoO_2N$	0.902291	0.36996453	N
$GaVO_2N$	0.879871	0.40486685	N
$GaNbO_2N$	0.838216	0.47467148	N
$GaTaO_2N$	0.838216	0.47467148	N
$GaMoO_2N$	0.850292	0.45373009	N
$GaWO_2N$	0.846229	0.46071055	N
$InSiO_2N$	1.027409	0.27921852	N
$InGeO_2N$	0.959341	0.36996453	N
$InSnO_2N$	0.887015	0.48165194	N
$InTiO_2N$	0.924023	0.42231801	N
$InZrO_2N$	0.874651	0.50259333	N
$InHfO_2N$	0.878734	0.49561287	N
$InMnO_2N$	0.959341	0.36996453	N
$InFeO_2N$	0.933184	0.40835708	N
$InCoO_2N$	0.959341	0.36996453	N
$InVO_2N$	0.935503	0.40486685	N
$InNbO_2N$	0.891214	0.47467148	N
$InTaO_2N$	0.891214	0.47467148	N
$InMoO_2N$	0.904054	0.45373009	N
$InWO_2N$	0.899733	0.46071055	N
$LaSiO_2N$	1.077573	0.27921852	N
$LaGeO_2N$	1.006181	0.36996453	N
$LaSnO_2N$	0.930324	0.48165194	P
$LaTiO_2N$	0.969139	0.422318	S/P
$LaZrO_2N$	0.917357	0.502593	S/P
$LaHfO_2N$	0.921639	0.49561287	P
$LaMnO_2N$	1.006181	0.36996453	N
$LaFeO_2N$	0.978748	0.40835708	P
$LaCoO_2N$	1.006181	0.36996453	N
$LaVO_2N$	0.981180	0.404867	S[a]/P
$LaNbO_2N$	0.934728	0.474671	P
$LaTaO_2N$	0.934728	0.474671	P
$LaMoO_2N$	0.948195	0.453730	P
$LaWO_2N$	0.943663	0.460711	P
$PrSiO_2N$	1.082976	0.27921852	N
$PrGeO_2N$	1.011225	0.36996453	N
$PrSnO_2N$	0.934988	0.48165194	P
$PrTiO_2N$	0.973998	0.422318	P
$PrZrO_2N$	0.921956	0.502593	S/P
$PrHfO_2N$	0.926259	0.49561287	P
$PrMnO_2N$	1.011225	0.36996453	N
$PrFeO_2N$	0.983654	0.40835708	P
$PrCoO_2N$	1.011225	0.36996453	N
$PrVO_2N$	0.986099	0.404867	P
$PrNbO_2N$	0.939414	0.474671	P
$PrTaO_2N$	0.939414	0.474671	P
$PrMoO_2N$	0.952949	0.453730	P
$PrWO_2N$	0.948394	0.460711	P
$NdSiO_2N$	1.042845	0.27921852	N
$NdGeO_2N$	0.973753	0.36996453	N
$NdSnO_2N$	0.900341	0.48165194	P
$NdTiO_2N$	0.937905	0.422318	S/P
$NdZrO_2N$	0.887791	0.502593	S/P
$NdHfO_2N$	0.891935	0.49561287	P
$NdMnO_2N$	0.973753	0.36996453	N
$NdFeO_2N$	0.947204	0.40835708	P
$NdCoO_2N$	0.973753	0.36996453	N
$NdVO_2N$	0.949557	0.40486685	S/P
$NdNbO_2N$	0.904603	0.47467148	P
$NdTaO_2N$	0.904603	0.47467148	P
$NdMoO_2N$	0.917636	0.45373009	P
$NdWO_2N$	0.91325	0.46071055	P
$SmSiO_2N$	1.031268	0.27921852	N

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$SmGeO_2N$	0.962944	0.36996453	N
$SmSnO_2N$	0.890346	0.48165194	N
$SmTiO_2N$	0.927493	0.42231801	N
$SmZrO_2N$	0.877936	0.50259333	S/P
$SmHfO_2N$	0.882034	0.49561287	N
$SmMnO_2N$	0.962944	0.36996453	N
$SmFeO_2N$	0.936689	0.40835708	P
$SmCoO_2N$	0.962944	0.36996453	N
$SmVO_2N$	0.939017	0.40486685	P
$SmNbO_2N$	0.894561	0.47467148	N
$SmTaO_2N$	0.894561	0.47467148	N
$SmMoO_2N$	0.907449	0.45373009	N
$SmWO_2N$	0.903112	0.46071055	N
$ABON_2$ $A^{2+}B^{6+}$			
$MgMoON_2$	0.91418	0.40248388	N
$MgWON_2$	0.909754	0.40930564	N
$CaMoON_2$	0.965085	0.402484	N
$CaWON_2$	0.960413	0.409306	P
$SrMoON_2$	0.999480	0.402484	N
$SrWON_2$	0.994641	0.409306	P
$BaMoON_2$	1.057951	0.402484	N
$BaWON_2$	1.052829	0.409306	N
$ZnMoON_2$	0.914984	0.40248388	N
$ZnWON_2$	0.910555	0.40930564	N
$CdMoON_2$	0.954766	0.40248388	N
$CdWON_2$	0.950144	0.40930564	P
$EuMoON_2$	0.998792	0.40248388	N
$EuWON_2$	0.993957	0.40930564	P
$A^{3+}B^{5+}$			
$ScVON_2$	0.901012	0.36837508	N
$ScNbON_2$	0.85822	0.43659269	N
$ScTaON_2$	0.85822	0.43659269	N
$ScMoON_2$	0.870625	0.4161274	N
$ScWON_2$	0.86645	0.42294916	N
$YVON_2$	0.957876	0.36837508	N
$YNbON_2$	0.912383	0.43659269	N
$YTaON_2$	0.912383	0.43659269	N
$YMoON_2$	0.925571	0.4161274	N
$YWON_2$	0.921133	0.42294916	N
$GaVON_2$	0.89455	0.36837508	N
$GaNbON_2$	0.852065	0.43659269	N
$GaTaON_2$	0.852065	0.43659269	N
$GaMoON_2$	0.864381	0.4161274	N
$GaWON_2$	0.860236	0.42294916	N
$InVON_2$	0.950367	0.36837508	N
$InNbON_2$	0.905231	0.43659269	N
$InTaON_2$	0.905231	0.43659269	N
$InMoON_2$	0.918315	0.4161274	N
$InWON_2$	0.913912	0.42294916	N
$LaVON_2$	0.996196	0.368375	N
$LaNbON_2$	0.948883	0.436593	S/P
$LaTaON_2$	0.948883	0.436593	S/P
$LaMoON_2$	0.962598	0.416127	P
$LaWON_2$	0.957983	0.422949	S^a/P
$PrVON_2$	1.001131	0.368375	N
$PrNbON_2$	0.953584	0.436593	S/P
$PrTaON_2$	0.953584	0.436593	P
$PrMoON_2$	0.967367	0.416127	P
$PrWON_2$	0.962729	0.422949	P
$NdVON_2$	0.964468	0.36837508	N
$NdNbON_2$	0.918663	0.43659269	N
$NdTaON_2$	0.918663	0.43659269	N
$NdMoON_2$	0.931941	0.4161274	P
$NdWON_2$	0.927472	0.42294916	S^a/P
$SmVON_2$	0.953892	0.36837508	N
$SmNbON_2$	0.908589	0.43659269	N
$SmTaON_2$	0.908589	0.43659269	N
$SmMoON_2$	0.921721	0.4161274	N
$SmWON_2$	0.917302	0.42294916	N

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